8TH ASIA OCEANIA CONFERENCE ON GREEN AND SUSTAINABLE CHEMISTRY

AOC-GSC8
CONFERENCE HANDBOOK

29 November – 1 December 2023
Auckland, New Zealand

CONTENTS

WELCOME

Tēnā koutou | Dear Colleague,

It is our pleasure to welcome you to the 8th Asia-Oceania Conference on Green and Sustainable Chemistry (AOC-GSC8). The AOC-GSC conference series is a biennial series with the goal of advancing green and sustainable chemistry within the Asia-Oceania region. Past editions of this conference series have been held in cities across the region including Tokyo (2007), Beijing (2009), Melbourne (2011), Taipei (2013), New Delhi (2015), Hong Kong (2016) and Singapore (2018). We are pleased to bring this conference to Aotearoa | New Zealand for the first time this year.

We are excited to see the range of topics that will be covered by speakers at this conference from energy applications, green synthesis and catalysis, toxicology, waste remediation and valorisation, the development of biobased products, green chemistry education, environmental policy and management alongside emerging chemical technologies such as flow chemistry and mechanochemistry. One of the aims of this conference series is to encourage the sharing of scientific knowledge and stimulate new collaborations across the region and we are particularly pleased to see the wide range of countries from the Asia-Oceania region and abroad which will be represented here.

Welcome to Tāmaki Makaurau | Auckland and thank you for joining us as every contribution helps to ensure AOC-GSC8 is a successful event.

Ngā manaakitanga | Best Wishes,

Cameron Weber and Jonathan Sperry

AOC-GSC8 Organising Committee

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GOLD

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AOC-GSC8 Programme

Wednesday 29th November

TIME	EVENT	LOCATION
09:30 - 15:00	Registration Opens	Engineering Building 405 Level 4 Foyer
10:00 - 11:00	Arrival Tea & Coffee	Engineering Building 405 Level 4 Foyer
11:00 - 11:30	Opening and Welcome	Lecture Theatre 401-401
11:30 - 12:30	**Plenary Session 1: John Warner** *Green Chemistry: The Missing Elements*	Lecture Theatre 401-401
12:30 - 13:30	Lunch	Engineering Building 405 Level 4 Foyer
13:30 - 14:00	**Keynote Session 1: Debabrata Maiti** *En-Lightening C-H Functionalization*	Lecture Theatre 401-401
	Oral Session 1	
	Lecture Theatre 401-401	**Lecture Theatre 401-439**
	Sustainable Agriculture and Pollutant Remediation	**Synthesis**
14:00-14:20	*New Frontiers in Polymers Made from Sulfur* **Justin Chalker**	*Computation and Experiment in Synergy: A Sustainable Research Approach* **Nadeem Sheikh**
14:20-14:40	*Regulation of plant ethylene biosynthesis for sustainable agriculture* **Ivanhoe Leung**	*Development of heterogeneous catalysts for hydrogenation of carboxylic acids* **Masazumi Tamura**
14:40-14:55	*Esterified Lignin Nanoparticles for Pesticide Delivery to Plant Leaves* **Matilda Andersson**	*Electrochemical oxidation of 3-substituted indoles* **Juan Arteaga Giraldo**
14:55-15:10	*Using the potential of waste biomass in the bioremediation of soil contaminated with heavy metal ions* **Izabela Michalak**	*Endo-selective 1,4-addition of thiols to (–)-levoglucosenone* **Atsushi Tahara**
15:10-15:25	*Removal of antibiotic residues in aqueous solutions using Polyvinyl alcohol-Glycine-Zirconium(IV)tungstophosphate (PVA-Gly-ZWP) Membrane* **Jitha Kunhikrishnan**	

15:25-16:00	Afternoon Tea	Engineering Building 405 Level 4 Foyer
	Oral Session 2	
	Lecture Theatre 401-401	**Lecture Theatre 401-439**
	Biomass	**Nanoparticles and Metal Clusters**
16:00-16:20	*Grape marc as a source of high-value products including antioxidant biopolymers* **Paul Kilmartin**	*Toward Greener Synthetic Routes to Gold and Silver Nanomaterials* **Michelle Regulacio**
16:20-16:40	*Sustainable Bioproducts to Promote a Circular Economy* **Colin Barrow**	*Precisely controlled single atom and nanocluster-based materials: from fundamentals to applications in catalysis and energy* **Vladimir Golovko**
16:40-16:55	*Extraction and Derivatisation of Hemicellulose for Novel Applications* **Antonio Patti**	*Development of metal nanoparticle catalysts modified using multidentate polyoxometalates* **Kang Xia**
16:55-17:10	*Psidium guajava (Guava) leaves ash: A green heterogeneous catalyst for efficient biodiesel production* **Ankita Sarkar**	*Development of High Entropy Alloy Subnanocluster Catalysts and its Structural Reversibility under Oxidative/reductive Conditions* **Naoki Hashimoto**
17:10-17:25	*Thermally insulating foams based on upcycled aramid nanofibers and nanocellulose* **Lennart Bergström**	*Atomically Dispersed Co-Ni Dual-Metal Sites Showing Unique Reactivity and Dynamics for the Oxygen Evolution Reaction* **Jun-Xi Wu**
17:25-17:40	*Hydrophobic pine bark extracts for the surface treatment of natural fibres* **Regis Risani**	
17:40-17:55	*Eco-friendly recovery of alginate, fucoidan, and phenolics via aqueous ball milling of brown seaweed* **Sachin Talekar**	
17:55-19:00	Welcome Reception	Engineering Building 405 Level 4 Foyer

Thursday 30th November

TIME	EVENT	LOCATION
08:30 - 09:00	Arrival Tea & Coffee	Engineering Building 405 Level 4 Foyer
09:00 - 10:00	**Plenary Session 2: Xiaonan Wang** *Harnessing AI for Green and Sustainable Chemistry towards Carbon Neutrality*	Lecture Theatre 401-401
10:00 - 10:30	**Keynote Session 2: Kei Saito** *Self-healing polymers from biobased compounds*	Lecture Theatre 401-401
10:30 - 11:00	Morning Tea	Engineering Building 405 Level 4 Foyer
	Oral Session 3	
	Lecture Theatre 401-401	**Lecture Theatre 401-439**
	Waste Utilisation	**Alternative Solvents and Catalysis**
11:00-11:20	*CO2-derived oxalic acid-assisted conversion of organic and inorganic resources* **Shinji Kudo**	*Quantifying reaction outcomes in ionic liquids* **Jason Harper**
11:20-11:40	*Computational prediction of the catalyst surface hydrogen coverage in the hydrogenolysis of plastic waste* **Martina Lessio**	*Amphiphilic Ionic Liquid cytotoxicity: structure-activity and mechanistic studies* **Tristan Rawling**
11:40-11:55	*Waste Plastics as Resources for Functional Material and Chemical Production* **Jason Lim**	*Sub- and supercritical fluids for the biomass conversion* **Jaehoon Kim**
11:55-12:10	*Fluorous Nanochannels Enabling Ultrafast Desalination* ***Shuo Chen***	*Hydroxide-ion induced efficient mineralization of poly(vinylidene fluoride) and related copolymers in subcritical water* **Hisao Hori**
12:10-12:25	*Evaluation of the microbial hydrogenotrophic methanation process for power to gas* **Byoung-in Sang**	*Catalytic decomposition of polypropylene in petroleum-based solvents* **Mahiro Matsushita**
12:25-13:30	Lunch	Engineering Building 405 Level 4 Foyer
	Oral Session 4	
	Lecture Theatre 401-401	**Lecture Theatre 401-439**
	CO2 Conversion	**Heterogeneous Catalysis**

13:30-13:50	*Direct Conversion of Low-Concentration of CO2 to Polyurethane Raw-Materials Using an Organic Base as CO2 Capture Agent* **Katsuhiko Takeuchi**	*Atomically Dispersed Metal Catalysts Steering Selective Electrocatalysis* **Sang Hoon Joo**
13:50-14:10	*Multi-scale modeling of the electrochemical CO2 reduction reaction: Challenges and opportunities* **Yu Mao**	*Chemocatalytic Synthesis of Amino Acids from Renewable Feedstock* **Yiying Xiao**
14:10-14:25	*Methanol Production by CO2 Hydrogenation Catalyzed by Dinuclear Iridium Complexes under Gas-Solid Phase Conditions* **Yuichiro Himeda**	*Synthesis of novel photocatalysts for hydrogen and oxygen production via water splitting* **Areef Billah**
14:25-14:40	*CO2-blown Non-isocyanate Polyurethane Foams* **Ping Choong**	*Mechanistic study on electro-oxidation of 5-hydroxymethylfurfural and water molecules via operando surface-enhanced Raman spectroscopy coupled with an Fe3+ probe* **Yongfang Zhou**
14:40-14:55	*Visible-light driven fumarate synthesis using CO_2 gas as a direct feedstock in a bio/photocatalytic hybrid system* **Mika Takeuchi**	*Polyethylene decomposition over zeolite catalysts in hydrocarbon solvents* **Masahiko Matsukata**
14:55-15:10	*Hydrocarbon synthesis from CO2 using spinel oxide and zeolite* **Kazuya Hashimoto**	
15:10-15:25	*Applications of computational chemistry in atmospheric science* **Sara Farahani**	
15:25-16:00	Afternoon Tea	Engineering Building 405 Level 4 Foyer
16:00 - 16:30	**Keynote Session 3: Laurel Schafer** *Green Chemistry Enabled Synthesis of Aminated Responsive Materials*	Lecture Theatre 401-401
16:30 - 17:00	**Keynote Session 4: Thomas Maschmeyer** *BTEX from Lignin using a Novel Molybdenum Carbo-nitride@Titanium Nitride Catalyst*	Lecture Theatre 401-401
17:00 - 19:00	Poster Session	Engineering Building 405 Level 4 Foyer

Friday 1st December

TIME	EVENT	LOCATION
09:00 - 09:30	Arrival Tea & Coffee	Engineering Building 405 Level 4 Foyer
	Oral Session 5	
	Lecture Theatre 401-401	**Lecture Theatre 401-439**
	Metal Clusters and Metal Organic Frameworks	**Synthesis**
09:30 - 09:50	*Shifting Catalytic Activity and Selectivity Atom-by-Atom by Subnanometer Cluster Catalysts* **Stefan Vajda**	*Catalytic Asymmetric Synthesis of Chiral Indole Derivatives* **Feng Shi**
09:50 - 10:10	*Addressing hydrocarbon separations using MOFs as a bottom-up approach towards energy alternatives* **Lauren Macreadie**	*Flow-enabled photosensitized [2+2] cycloadditions for the synthesis of natural products* **Zoe Wilson**
10:10 - 10:25	*Photocatalytic Hydrogen Peroxide Production Utilizing Al-Based Metal-Organic Frameworks* **Zheng Niu**	*Highly Active and Chemoselective Homobimetallic Ruthenium Catalyst for One-pot Reductive Amination in Water* **Gopal Deshmukh**
10:25 - 11:00	Morning Tea	Engineering Building 405 Level 4 Foyer
11:00 - 11:30	**Keynote Session 5: Mageswary Karpudewan** *Green Chemistry Education: A Fundamental Theoretical Perspective with Augmented Reality Integration for Enhanced Delivery*	Lecture Theatre 401-401
	Oral Session 6	
	Lecture Theatre 401-401	**Lecture Theatre 401-439**
	Synthesis and Green Chemistry Education	**Energy**
11:30- 11:50	*Green chemistry in higher education: An upstream approach to addressing sustainable development goals* **Amy Cannon**	*Study of Decarbonisation on the Special Remote Area in East Indonesia* **Eniya Listiani Dewi**
11:50- 12:10	*Temperature control strategy in a flow reactor for safer operation and higher heat efficiency* **Yosuke Muranaka**	*Molecular electron acceptors and the new photophysical landscape of organic solar cells* **Paul Hume**
12:10- 12:25	*Applied research in green and sustainable chemistry: a Singapore story* **Valerio Isoni**	*Electrolyte Design and Synthesis for Sodium-Ion Batteries* **Darren Ould**

12:25 - 14:00	Lunch	Engineering Building 405 Level 4 Foyer
	Lecture Theatre 401-401	**Lecture Theatre 405-422**
13:00-14:00	AON-GSC Meeting	Student Quiz
	Oral Session 7	
	Lecture Theatre 401-401	**Lecture Theatre 401-439**
	Energy, Separations and Metal Organic Frameworks	**Catalysis and Mechanochemistry**
14:00-14:20	*Regulating Lithium Metal Interfaces to Enhance the Cycle Life of Anode-free Lithium Metal Batteries* **Dong Jun Kim**	*Modular assembly of biomimetic catalysts from amphiphilic precursors* **Jack Chen**
14:20-14:40	*Exploring the potential for ionic liquid derived bio-degradable and bio-compatible proton conducting membranes* **Patricia Hunt**	*Using TSE as a Route to Sustainable Manufacture* **Deborah Crawford**
14:40-14:55	*High-pressure H2 and CO2 Production from Formic Acid* **Hajime Kawanami**	*Remarkable Catalytic Activity of Molybdenum Complexes Bearing 4-[3,5-Bis(trifluoromethyl)phenyl]pyridine-Based PNP-Type Pincer Ligand toward Ammonia Formation* **Taichi Mitsumoto**
14:55-15:10	*Poly(3-hexylthiophene)-based Graft Copolymers for Smart Self-transform Novel Transient Electronics* **Xin Sun**	*Ball Milling as a Scalable Destruction Technology for Toxic 'Forever Chemicals'* **Kapish Gobindlal**
15:10-15:25	*Eco-friendly oxygen reduction reaction electrocatalyst for high-performance green biofuel cells* **Edwin Nyangau**	*The Origin of the Waterfall Effect: The Earliest Known Example of On-Water Chemistry.* **Alexander Yuen**
15:25 - 16:00	Afternoon Tea	Engineering Building 405 Level 4 Foyer
16:00-17:00	**Plenary Session 3: Magda Titirici** *Sustainable Materials for Energy Storage and Conversion*	Lecture Theatre 401-401
17:00-17:30	Closing Ceremony (including prize giving)	Lecture Theatre 401-401
18:30 - 23:00	Conference Dinner	Maritime Room (Princes Wharf, Viaduct Harbour)

PLENARY SPEAKERS

Professor John Warner is one of the founders of the field of green chemistry, co-authoring the defining text “Green Chemistry: Theory and Practice” and articulating the 12 principles of green chemistry with Paul Anastas. He is a chemistry inventor who works to design and create commercial technologies inspired by nature consistent with the principles of green chemistry.

With nearly 350 patents, he has invented solutions for dozens of multinational corporations. His inventions have also served as the basis for several new companies (ALS therapy, hair color restoration, asphalt warm mix rejuvenators, low light indoor photovoltaics and water harvesting). He has over 100 publications providing foundational work in the fields of noncovalent derivatization, polymer photochemistry, metal oxide semiconductors and synthetic organic chemistry.

John has received prestigious awards as an academic (Presidential Award for Excellence in Science Mentoring – President G. W. Bush & NSF, 2004) and the August Wilhelm von Hofmann Medal from the German Chemical Society, 2022, industrial chemist (Perkin Medal – Society of Chemical Industry, 2014), inventor (Lemelson Ambassadorship – Lemelson Foundation & AAAS) and for governmental chemicals policy (Reinventing Government National Performance Review – Vice President A. Gore & EPA, 1997).

Professor Xiaonan Wang is currently an associate professor in the Department of Chemical Engineering at Tsinghua University. She received her BEng from Tsinghua University in 2011 and PhD from University of California, Davis in 2015. After working as a postdoctoral research associate at Imperial College London, she joined the National University of Singapore (NUS) as an assistant professor since 2017 and later became an adjunct associate professor. Her research focuses on the development of intelligent computational methods including multi-scale modelling, optimization, data analytics and machine learning for applications in advanced materials, energy, environmental and manufacturing systems to support smart and sustainable development. She is leading a Smart Systems Engineering research group at Tsinghua and NUS of more than 20 team members as PI and also led the Artificial Intelligence for Accelerated Materials Development programs in China and Singapore. She has published more than 140 peer-reviewed papers with an H-index of 41, organized and chaired several international conferences, and delivered more than 60 presentations and invited talks at conferences and universities on five continents. She is an associate editor and editorial board member of 10 SCI journals e.g., Applied Energy, Advanced Intelligent Systems. She was recognized as a World’s Top 2% Scientists, ACS Sustainable Chemistry & Engineering Lectureship Award Winner, AIChE-SLS Outstanding Young Principal Investigator, IChemE Global Awards Young Researcher finalist and selected for Royal Society International Exchanges Award, as well several best paper awards at IEEE and Applied Energy conferences and journals. She is also a program lead of the Association of Pacific Rim Universities (APRU)’s Sustainable Waste Management Program and advisory board member of several international organizations.

Professor Magda Titirici is a Chair in Sustainable Energy Materials in the Department of Chemical Engineering at Imperial College London. She is also a RAEng Chair in Emerging Technologies. Prior, Magda was a reader and professor at Queen Mary University of London and an independent group leader at the Max-Planck Institute of Colloids and Interfaces. Magda obtained her PhD from University of Dortmund in Germany.

Her research interests are related to the sustainable production of advanced materials from waste streams and their application in energy storage and conversion technologies. Her work is cited over 40.000 times and has been recognised with several awards from the Royal Academy of Engineering, Royal Society, Royal Society of Chemistry, Institute of Materials and Mines, etc.

KEYNOTE SPEAKERS

Professor Debabrata Maiti received his PhD from Johns Hopkins University in 2008 under the supervision of Prof. Kenneth D. Karlin. After postdoctoral studies at MIT with Prof. Stephen L. Buchwald, he joined the Department of Chemistry at IIT Bombay in 2011. His research interests are focused on the development of new and sustainable synthetic and catalytic methodologies. Currently he is an Associate Editor of *Journal of Organic Chemistry*.

Professor Kei Saito is currently a Professor, Graduate School of Advanced Integrated Studies in Human Survivability, Kyoto University, Japan. Before joining Kyoto University in Oct 2020, he was a tenured Associate Professor (2019-2020), Senior Lecturer (2016-2018), and Lecturer (2007-2015) at School of Chemistry, Monash University, Australia and JST PRESTO researcher (2015-2019), Japan. Before then, a Postdoctoral Fellow at the Centre for Green Chemistry, University of Massachusetts Lowell, USA (2005-2007) and a Visiting Research Associate at the Graduate School of Science and Engineering and at the Faculty of Science and Engineering at Waseda University, Japan (2004-2005). He studied Green Chemistry from one of the founders of Green Chemistry, Prof. John Warner, while he was at University of Massachusetts Lowell and was the member of the ARC Special Research Centre for Green Chemistry at Monash University.

The focus of his current research relates to the innovative development of new synthetic methods for the production of novel sustainable polymeric materials, based on the principles of Green Chemistry and the utilisation of these materials in a variety of industrial applications. Prof. Saito was elected as a Fellow of the Royal Society of Chemistry (UK) for his achievements in 2018. He has supervised 22 PhD students to completion until now.

Professor Laurel L. Schafer is in the Department of Chemistry at the University of British Columbia and is a Tier 1 Canada Research Chair in Catalyst Development. She received her BSc from the University of Guelph in 1993 and her PhD from the University of Victoria in 1999. She then went on to the University of California-Berkley to complete an NSERC post-doctoral fellowship with Prof. T. D. Tilley. Her research features Green Chemistry approaches to develop catalysts for atom-economic catalysis to prepare amines, N-heterocycles, and amine-containing polymers of relevance to the fine-chemical, polymer, pharmaceutical and agrochemical industries. She is a co-founder of a start-up company, A2O Advanced Materials that is commercializing catalytic and materials science technologies developed in her lab. She has received numerous awards for her work, including a Schlenk Lecture Award from the University of Tübingen (2021), a Green Chemistry Award from the Canadian Society for Chemistry, a von Humboldt Research Award, a Killam Research Fellowship, and a Killam Award for Graduate Student Mentorship. She is a Fellow of the Royal Society of Canada, the American Association of the Advancement of Science and the Royal Society of Chemistry.

Professor Thomas Maschmeyer is a professor of Chemistry at the University of Sydney, Founder of the London-listed Gelion plc (GELN), an energy storage company, and co-founder of the waste upcycler Licella Holdings. After completing his PhD in 1994 he went on to hold positions at the Royal Institution of Great Britain, the University of Cambridge, and the TU Delft's Institute of Chemical Technology before returning to the University of Sydney as an ARC Federation Fellow. He is Fellow of three Academies and has received numerous prizes and awards, most recently receiving the 'Australian Prime Minister's Prize for Innovation' across all technologies and the Australian Academy of Science's David Craig Medal, its highest award in chemistry. His research interests cover catalysis and sustainable processes, renewable and circular feedstocks (waste biomass/plastics), green hydrogen, ionic liquids, micro- and mesoporous nanostructured material and reversible energy-storage devices. Mura Technology has licenced Licella's plastic conversion technology and is engaged in a global rollout with Dow, KBR, Mitsubishi Chemicals, LGChem and Chevron Phillips. Dow has committed to five 125 ktps plants alone.

Professor Mageswary Karpudewan is an accomplished educator and researcher in the School of Educational Studies at University Sains Malaysia (USM). She obtained her PhD in Chemistry Education from USM in 2010. Her doctoral research focused on integrating green chemistry into the pre-service chemistry teachers' curriculum, which has since been widely recognized and cited globally as a reference point for expanding green chemistry into education.

Her work has gained theattention of several leading organizations, including the Green Chemistry Institute, American Chemistry Society, United Nations Environmental Program, and Beyond Benign, based in the US, other countries, such as Thailand, Indonesia, Philippines, and Germany. Her work also received most prestigious awards for integrating sustainability into education from UNESCO and American Chemistry Society. Besides green chemistry, due to the importance of introducing interdisciplinary perspective to science and chemistry education, she is continuously researching on teaching and learning of climate change and STEM education.

She is a globally renowned expert in research methodology, with expertise in quantitative, qualitative, and mixed-method research. Her proficiency in research methodology is evidenced by the numerous high impact publications she has produced. Additionally, she has been the principal consultant for various research method workshops that have been attended by participants from diverse fields, including social science, engineering, and medical sciences.

SPEAKER ABSTRACTS

PLENARY SESSION 1, LECTURE THEATRE 401-401, 29 NOVEMBER, 2023, 11.30 AM – 12.30 PM

Green Chemistry: The Missing Elements

John C. Warner

The Technology Greenhouse, LLC, 100 Tradecenter Suite 325, Woburn, MA 01801 USA

Imagine a world where all segments of society demanded environmentally benign climate neutral products! Imagine if all consumers, all retailers, and all manufacturers insisted on buying and selling only non-toxic truly sustainable materials! The unfortunate reality is that, even if this situation were to occur, our knowledge of materials science and chemistry wouldallow us to provide only a small fraction of the necessary products and materials that our economy is based upon. Unfortunately, the way we learn and teach chemistry and materialsscience in academia is for the most part void of any information regarding mechanisms of toxicity and environmental harm. Green Chemistry is a science that seeks to reduce or eliminate the use of hazardous materials at the design stage of a materials process. It has been demonstrated that materials and products CAN be designed with negligible impact on human health and the environment while still being economically competitive and successfulin the marketplace. This presentation will describe the history and background of Green Chemistry and discuss the opportunities for the next generation of materials designers to create a safer and more sustainable future.

KEYNOTE SESSION 1, LECTURE THEATRE 401-401, 29 NOVEMBER, 2023, 1.30 – 2.00 PM

En-Lightening C-H Functionalization

Debabrata Maiti

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The scientific community has long sought to emulate nature's mechanisms, particularly in understanding how enzymes achieve chemical transformations with precision. Through extensive research, we have gained a thorough understanding of how enzymes catalyze the functionalization of inert C–H bonds in a regio- and stereoselective manner, utilizing metal-active sites. Taking inspiration from these natural processes, we have successfully developed catalytic methods for the functionalization of carbon–hydrogen (C–H) bonds. The Fujiwara–Moritani reaction is one of such reaction which made significant impact on the development of modern C–H activation methodologies. Despite the traditional approach's widespread applicability in various fields, issues related to reactivityand regioselectivity have limited its effectiveness. To revive this remarkable reaction, it is necessary to establish a mechanistic framework that allows simultaneous control over both reactivity and regioselectivity. The conventional high-temperature conditions required for olefination often lead to undesired multiple functionalizations at different sites.

In our work, we have successfully established a photoredox catalytic system by merging a palladium catalyst with an organo-photocatalyst (PC). This innovative system enables selective oxidative olefination of diverse arenes and heteroarenes in a highly regioselective manner. The utilization of visible light plays a crucial role in driving these "regioresolved" Fujiwara–Moritani reactions, eliminating the need for silver salts and high thermal energy. Our catalytic system also exhibits compatibility with both proximal and distal olefination, facilitated by the appropriate directing groups (DGs). This versatility allows us to engage the entire spectrum of C(sp^2)–H olefination. The broad scope of this protocol allows for the synthesis of diverse compounds, including natural products, chiral molecules, and drugs. The established mechanistic insights further enhance our understanding of this reaction, enabling future advancements in this field. Importantly, this method offer significant advantages over traditional synthetic approaches, both in terms of economic feasibility and environmental impact.

Recent References

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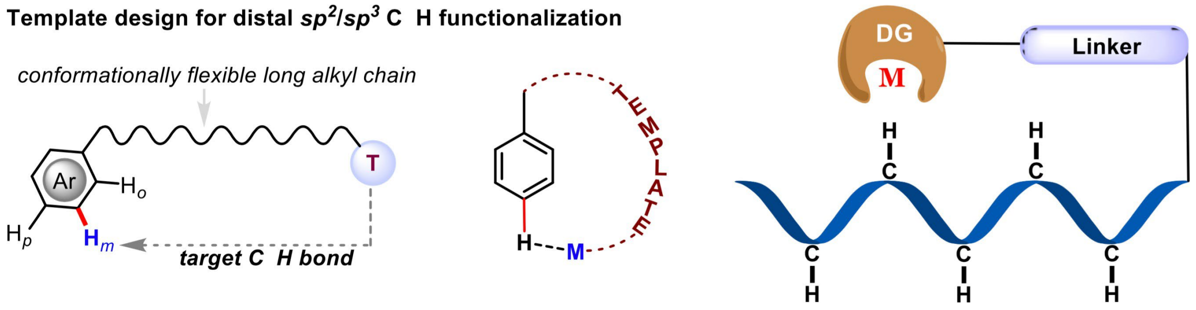

ORAL SESSION 1, LECTURE THEATRE 401-401, 29 NOVEMBER, 2023, 2.00 – 2.20 PM

New Frontiers in Polymers Made from Sulfur

Professor Justin M. Chalker[1]

[1] *College of Science and Engineering, Flinders University, Bedford Park, South Australia, Australia 5042*

Sulfur is an abundant feedstock generated in millions of tonnes each year in petroleum refining. Converting this sulfur into useful polymers is one way to repurpose this surplus industrial product (1). In our laboratory, the overarching goal is to use these polymers in applications that benefit the environment and human well-being (2,3). In this presentation, I will discuss design principles for making these sulfur polymers with tailored thermal, mechanical, and optical properties (4, 5). I will then present case studies in using these polymers as repairable and recyclable materials (6-7), next-generation lenses for thermal imaging (8), and versatile sorbents for pollution and precious metals (7,9).

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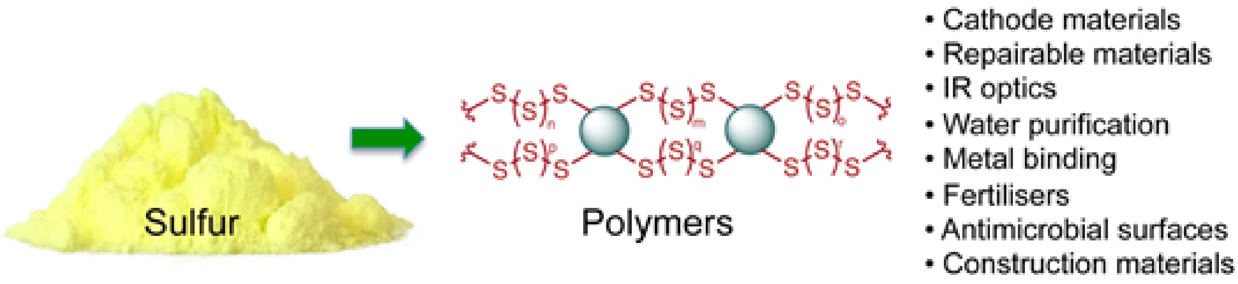

Figure: *Sulfur copolymers are useful in a variety of applications that benefit the environment and human well-being*

ORAL SESSION 1, LECTURE THEATRE 401-401, 29 NOVEMBER, 2023, 2.20 – 2.40 PM

Regulation of plant ethylene biosynthesis for sustainable agriculture

Dona M. Gunawardana,[1] Francis Kuang,[2] Simranjeet Kaur,[1] Davide Mercadante,[1] Michael J. Haydon,[3] Ivanhoe K. H. Leung[1,2]

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Extreme weather events and rising global temperatures caused by climate change are putting plants under increasing stress and pressure. These affect plant growth and development, threaten plant biodiversity and compromise crop yields. In this talk, I will reportour recent progress in studying the mechanism that plants use to modulate the biosynthesis of ethylene, a vital phytohormone that regulates the response of higher plants to environmental stress. Our results suggest that the plant ethylene-forming enzyme may undergo redox-mediated modifications that alter its function and activity both *in vitro* and *in planta*. As plant ethylene biosynthesis is intimately linked to plant growth and plant stress responses, our study provides important new knowledge that may be used to boost future crop productivity for sustainable agriculture.

ORAL SESSION 1, LECTURE THEATRE 401-401, 29 NOVEMBER, 2023, 2.40 – 2.55 PM

Esterified Lignin Nanoparticles for Pesticide Delivery to Plant Leaves

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The rapidly growing world population, expected to reach 9.7 billion by 2050, necessitates increased agricultural production,[1] leading to a higher use of pesticides. However, it is already known that the current use of pesticides is negatively affecting the nearby environment, thus threatening both biodiversity and human health.[2]

Therefore, we aim to develop hybrid nanocarriers made by combining kraft lignin and non-food long-chained fatty acids as a delivery system for an efficient use of pesticides. These two components are existing byproducts from biobased industries. Kraft lignin, obtained from the black liquor in kraft pulping[3] possesses antimicrobial[4] and UV-resistant properties,[3] is a carbon source for soils,[5] and has numerous active functional groups,[3] making it ideal for developing biobased plant protection systems. Herein esterified kraft lignin was used to synthesise spherical nanoparticles with a hydration barrier composed of the fatty acid chains, as previously reported by our group.[6] Our current focus aims to evaluate the adhesion forces between theparticles and epicuticular wax present on surfaces of plant leaves. This way, we attempt to ensure UV-barrier for photodegradable pesticides, while achieving sufficient stability and site-specific release of the cargo under different weather conditions.

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ORAL SESSION 1, LECTURE THEATRE 401-401, 29 NOVEMBER, 2023, 2.55 – 3.10 PM

Using the potential of waste biomass in the bioremediation of soil contaminated with heavy metal ions

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Heavy metals are currently one of the most significant environmental pollutants. Soil contaminated with toxic metals is a global problem, since they pose a threat to the healthand life of all living organisms. In particular, plants have a high capacity to accumulate toxic metals present in the soil in their biomass. Therefore, it is necessary to take actions aimed atlimiting the bioaccumulation of these elements in plants, increasing plant production and ensuring the safety of the food produced. This study proposes the use of waste biomass, such as sawdust, to immobilize contaminants in the polluted soil, thereby limiting their bioavailability to plants. This biomass has the ability to bind metal ions due to its biosorption properties, which have been tested in relation to Pb(II), Cr(III), Zn(II), Cd(II) and Cu(II) ions. Experiments on kinetics and equilibrium of biosorption of these metal ions were carried out. Prior this process, the tested biosorbents have been characterized in detail using a number of techniques, such as: multielement analysis by ICP-OES, CHNS, XRF techniques, thermogravimetric analysis, SEM-EDX and FTIR. The effectiveness of this biosorbent as a heavy metal immobilizing agent was confirmed in pot tests carried out using contaminated soil and winter wheat as a model plant. In the control group, the classic phytoremediation process was used. The proposed solution may enable the cultivation of plants in contaminated areas and at the same time may be a sustainable way to manage waste biomass.

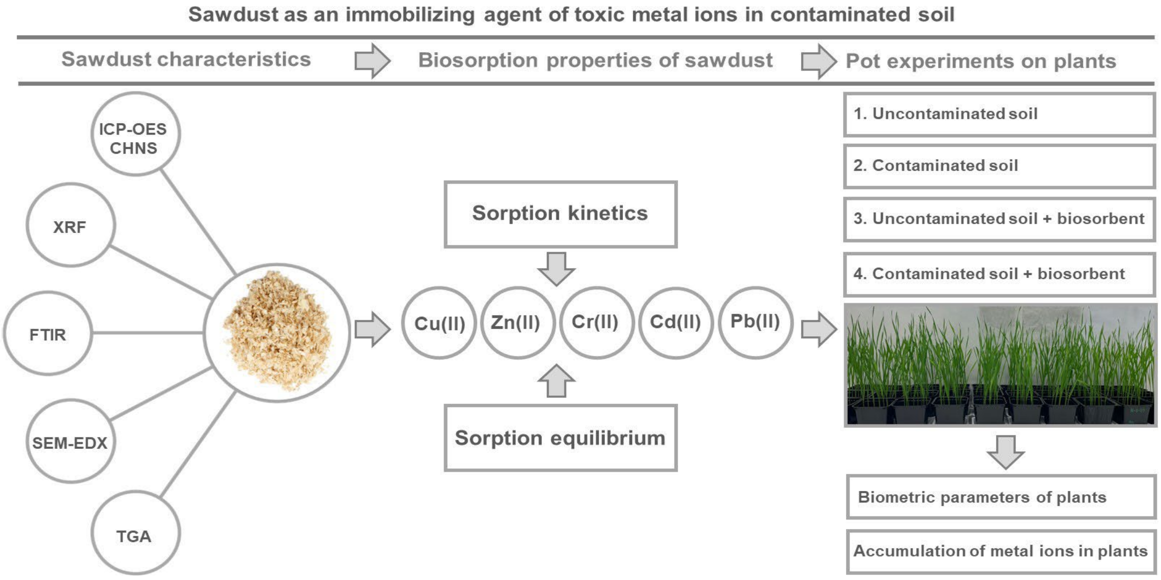

Figure 1: *Research methodology*

Acknowledgements

This research was performed in the framework of the project entitled "Biomass valorizationto enhance efficiency of toxic metals bioremediation from military and industry areas" financed by OPCW (No: L/ICA/ICB-105/21, The Hague, The Netherlands, 31.12.2021–31.12. 2023).

ORAL SESSION 1, LECTURE THEATRE 401-401, 29 NOVEMBER, 2023, 3.10 – 3.25 PM

Removal of antibiotic residues in aqueous solutions using Polyvinyl alcohol-Glycine-Zirconium(IV)tungstophosphate (PVA-Gly-ZWP) Membrane

Charishma Ravindran[1], Jitha Kunhikrishnan Maniath[2], Anitha Panayam Parambil Kunnathulli[3]

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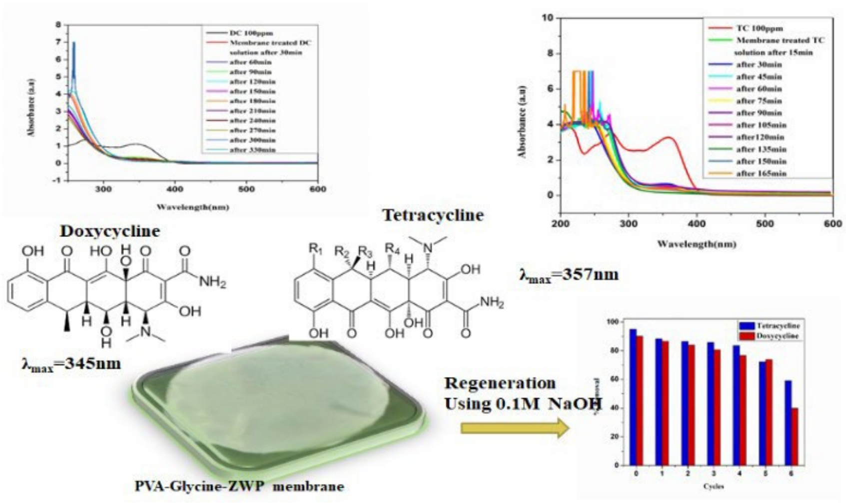
The serious problem of excess antibiotic usage and release into our environment has to be considered under immediate action. Antibiotic residues induce antibiotic resistance among microorganisms and thereby they create a threat of incurable dreadful diseases. An easy method to rectify the problem is to discard the residue from pharma waste and other waste streams which are primary sources of antibiotic residues. The current study deals with the removal of two antibiotic- residues (tetracycline and doxycycline) at a time using a newly fabricated polymer composite filtration membrane of Polyvinyl alcohol (PVA), Glycine (Gly), and with an ion exchanger as filler. The addition of filler - Zirconium(IV)tungstophosphate (ZWP) enhanced the performance of the membrane for the purpose. The PVA-Gly-ZWP membrane was characterized by XRD, FTIR, SEM-EDX, TGA-DTA and UV-Visible spectrophotometer, contact angle goniometer etc. Adsorption behavior of membranes towards TC and DC were carried out using a batch adsorption system. The concentration of TC and DC was measured by UV-Visible spectrophotometer at a maximum wavelength of 357nm and 345nm, respectively. The optimum pH for the removal of both antibiotics was found to be 6. The filtration studies showed that the flux of membrane increased from 73.38±22.39L/m^2h to 106.79±13.73L/m^2h. A retention of about 70% were obtained for both the antibiotics simultaneously with bare membrane. But about 98% retention was observed when the feed was pretreated with activated charcoal. The maximum adsorptive removal rate of 94.89% for TC and 90.24% for DC using PVA-Gly-ZWP membrane was observed in the batch adsorption process. As a theoretical approach, the nature and extent of adsorption were evaluated by kinetic, isotherm and thermodynamic studies. Pseudo second order kinetic model and Langmuir isotherm models fits significantly more than that of other models. Regeneration of TC and DC adsorbed membranes were successfully done using sodiumhydroxide showing the reusability of the membrane.



ORAL SESSION 1, LECTURE THEATRE 401-439, 29 NOVEMBER, 2023, 2.00 – 2.20 PM

Computation and Experiment in Synergy: A Sustainable Research Approach

Nadeem S. Sheikh[1]

[1]*Chemical Science, Faculty of Science, Universiti Brunei Darussalam, Brunei Darussalam*

Computational chemistry is the most relevant field to predict the reactivity and selectivity of an organic reaction and computational investigation has become a commonplace in chemical synthesis. A judicious application of integrated synthetic and theoretical approach is highly beneficial because computational study allows the determination of crucial features of a chemical synthesis, which are very challenging to monitor *via* conventional synthetic processes. In short, both computational and synthetic domains of research nicely complement with each other to facilitate the scientific community. Taking an advantage of this synergistic research approach, we have demonstrated its application towards visible- light-mediated photoredox catalysis.[1] This collaborative work provides a very powerful platform for the divergent assembly of poly-functionalized bioactive nitrogen heterocycles and late-stage modification of blockbuster drug molecules (**Figure 1**). For this photocatalytic transformation, computational studies have unequivocally shed light on several parameters that affect the reactivity, especially in the case of polarised processes. In addition to this, we have applied computational studies in the field of nanomaterials and to investigate the torquoselectivity and captodative substitution induced acceleration effect towards pericyclic transformations.[2] This highlights some interesting reactivity features, which can lead to an efficient and sustainable computer-aided synthetic design for preparation of bioactive organic molecules and valuable materials.

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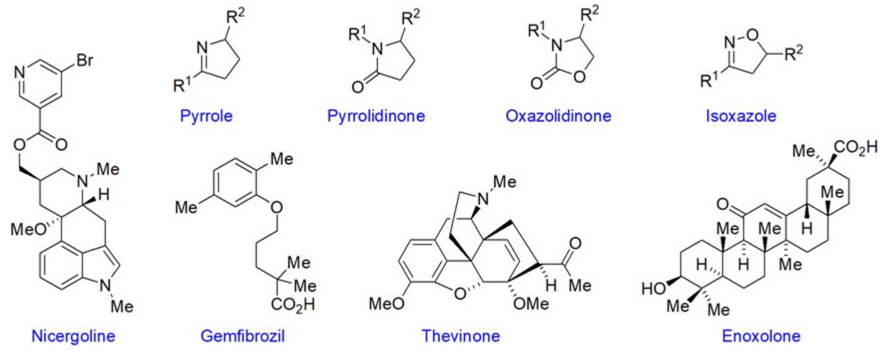

***Figure 1**: Computation and experiment in synergy: Synthesis of heterocycles and late-stage modifications of potent molecules.*

ORAL SESSION 1, LECTURE THEATRE 401-439, 29 NOVEMBER, 2023, 2.20 – 2.40 PM

Development of heterogeneous catalysts for hydrogenation of carboxylic acids

Masazumi Tamura
Osaka Metropolitan University, Graduate School of Engineering, Osaka, Japan

Hydrogenation of carboxylic acids is an important organic reaction for the synthesis of various alcohols, and versatile effective homogeneous and heterogeneous catalysts have been developed up to now [1]. In terms of the reusability and durability of catalysts, heterogeneous catalysts are preferable to homogeneous ones in the industry. In our research groups, we have developed heterogeneous catalysts for the hydrogenation of various carboxylic acids such as fatty acids, lactic acid, amino acids, and so on, and reported that the combination catalysts composed of metal oxides and noble metals and alloy catalysts are effective heterogeneous ones at comparatively low reaction temperatures (≤413 K) (Figure 1): Re-Pd/SiO_2 for hydrogenation of fatty acids and diacids to fatty alcohols and diols, respectively [2], Mo-Pt alloy in Mo-Pt/SiO_2 for hydrogenation of fatty acids to fatty alcohols [3], Rh-MoO_x/SiO_2 for hydrogenation of amino acids to amino alcohols [4], Ru- MoO_x/SiO_2 or Ru-MoO_x/C for hydrogenation of lactic acid to 1,2- propane diol [5]. In this presentation, the details of the catalyst systems for each hydrogenation reaction will be introduced including the recently developed catalyst system, and the catalyst design for the hydrogenation reactions will be discussed.

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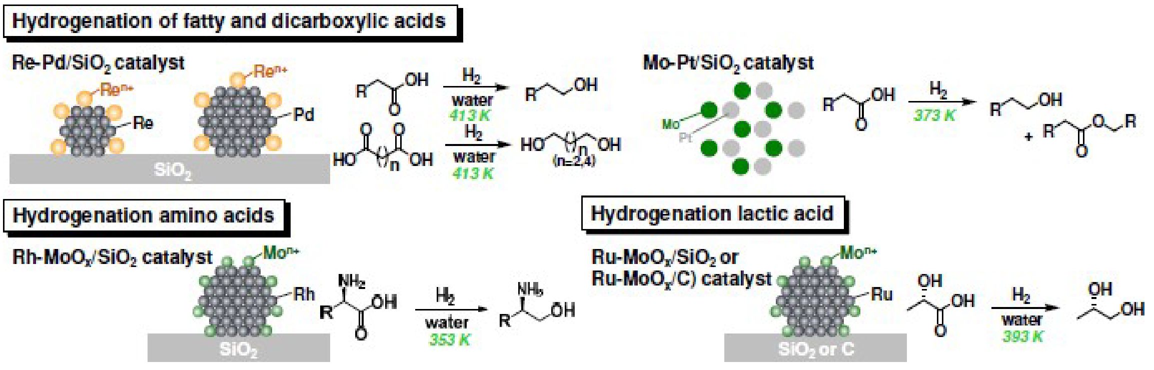

Figure 1: *Hydrogenation of carboxylic acids by the combination catalyst of metal oxides and noblemetals and alloy catalysts*

ORAL SESSION 1, LECTURE THEATRE 401-439, 29 NOVEMBER, 2023, 2.40 – 2.55 PM

Removal of antibiotic residues in aqueous solutions using Polyvinyl alcohol-Glycine-Zirconium(IV)tungstophosphate (PVA-Gly-ZWP) Membrane

Electrochemical oxidation of 3-substituted indoles

Juan J. Arteaga Giraldo, Ashley C. Lindsay, Rachel Chae-Young Seo, Paul A. Kilmartin, Jonathan Sperry

Centre for Green Chemical Sciences, School of Chemical Sciences, The University ofAuckland

2-Oxindoles are privileged heteroaromatic compounds that are found in a variety of biologically active natural products and pharmaceuticals.[1] Due to the biological activity present on the oxindole core, a large body of research has focused on constructing this heterocycle. The most straightforward approach is the direct oxidation of the parent indole,[2-6] however, this transformation requires the stoichiometric use of chemical oxidants, which present safety and environmental hazards and downstream purification issues. Herein, we report that 3-substituted indoles undergo an electrochemically mediated oxidation to the corresponding 2-oxindole in the presence of potassium bromide (KBr). Cyclic voltammetry and control studies infer that the reaction proceeds by electrochemical generation of elemental bromine (Br_2) that, upon reaction with indole, followed by hydrolysis, delivers the

2-oxindole. This procedure is an appealing alternative to chemical oxidants in the synthesisof 2-oxindoles by oxidation of the parent indole.

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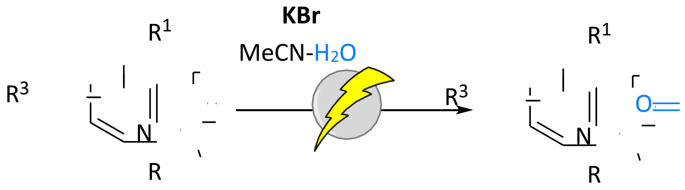

Figure: Electrochemically mediated oxidation of indoles to 2-oxindoles

ORAL SESSION 1, LECTURE THEATRE 401-439, 29 NOVEMBER, 2023, 2.55 – 3.10 PM

Endo-selective 1,4-addition of thiols to (–)-levoglucosenone

Atsushi Tahara,[1,2] Reo hasegawa[2], Shinji Kudo,[3] Yoshihito Shiota,[3] Takayuki Doi[2]

[1]Frontier Research Institute for Interdisciplinary Sciences (FRIS), Tohoku University.[2]Graduate School of Pharmaceutical Sciences, Tohoku University.

[3]Institute for Materials Chemstry and Engineering, Kyushu University.

(–)-Levoglucosenone [(–)-LGO] is one of enantiomerically pure anhydrosugars obtained from acid-catalyzed pyrolysis of cellulose via the formation of an intramolecular 1,6-glycosidic bond. A Structural feature of (–)-LGO is a rigid oxabicyclo[3,2,1]octane skeleton having an □,□-unsaturated ketone and a cyclic acetal. (–)-LGO has been used not only as a chiral building block but also a biomass feedstock. It was also reported that (–)-LGO and its derivatives showed cytotoxicity toward several cancer cell lines. Due to steric hindrance by the cyclic acetal, most addition reactions to □,□-unsaturated ketone of (–)-LGO proceeds stereoselectively. For example, 1,4-addition reaction of thiols, amines and alcohols to (–)- LGO gave *exo*-adducts selectively, so as epoxidation and Diels-Alder reaction.[1] In contrast,there have been no reports about direct formation of *endo*-adducts, except for one exampleby sequential treatment of (–)-LGO with iodobenzene in the presence of Pd catalyst (Heck reaction) followed by *exo*-selective hydrogenation with H_2.[2] We herein report *endo*-selective1,4-addition of thiols to (–)-LGO by controlling thermodynamic stability of the products.

Optimization of reaction conditions, substrate scopes and limitations, application of the resulting *endo*-adducts (cytotoxicity toward several cancer cell lines) will also be presented.

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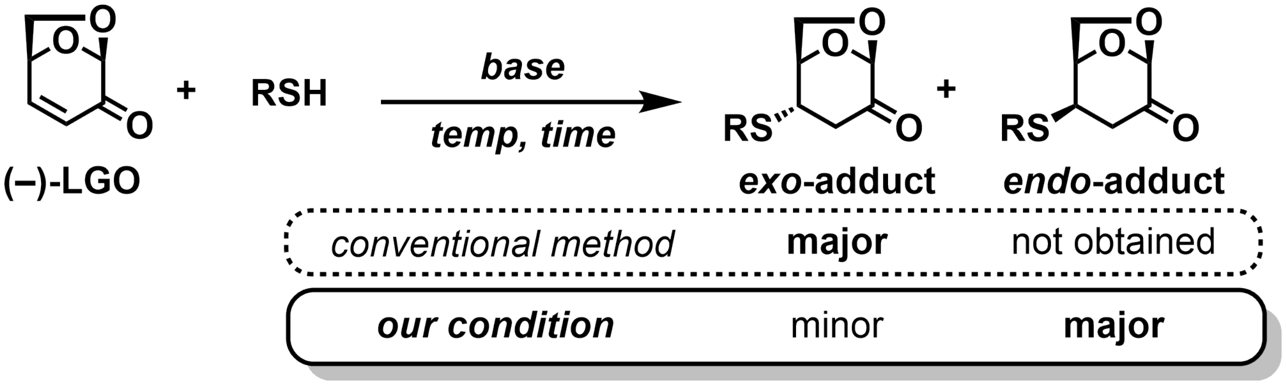

Figure: *classilcal (exo-selective) and non-classical (endo-selective) 1,4-addition reaction of thiols to (–)-levoglucosenone.*

ORAL SESSION 2, LECTURE THEATRE 401-401, 29 NOVEMBER, 2023, 4.00 – 4.20 PM

Grape marc as a source of high-value products including antioxidant biopolymers

Paul A. Kilmartin[1]

[1]*Centre for Green Chemical Science, School of Chemical Sciences, University of Auckland, New Zealand*

Grape marc is a source of useful compounds that can be used to create new high-value products, including biopolymers for food packaging applications [1]. Tannins present within acommercial grape seeds powder (437 mg gallic acid per g), or a grape skins solution (14 mg gallic acid per g) were added into gelatin to create biopolymer films with active and intelligent properties [2]. Both tannin extracts displayed differences in colour in solution as the pH was changed, which provided an intelligent function with the use of skin tannins [3]. The films released a proportion of the tannins into a 50% ethanolic food simulant, and exhibited antioxidant activity, given by the DPPH radical scavenging by the same food simulant, particularly the films containing grape seed tannins.

This project will continue as part of a recently funded MBIE programme (2023 to 2028), "*Waste to treasure: using novel chemistry to valorise residual plant materials*", involving researchers from the University of Auckland, Scion, University of Canterbury and Auckland University of Technology. The programme will use grape marc waste fractions that have received little attention in the past, including grape proteins and bioactive polyphenols suitable for the food industry, fine chemicals and surfactants, along with high-value paper products with fire-retardant and antimicrobial properties and paper-based electronics. The research is directed to eliminating a problem horticultural waste stream and will help to establish economically and environmentally sound local biorefineries.

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ORAL SESSION 2, LECTURE THEATRE 401-401, 29 NOVEMBER, 2023, 4.20 – 4.40 PM

Sustainable Bioproducts to Promote a Circular Economy.

Colin J. Barrow

[1]*Centre for Sustainable Bioproducts, Deakin University, Waurn Ponds, VIC 3216, Australia*

Food, agricultural and marine sectors are important contributors to the Australian economy but generate vast quantities of underutilized biomass which is often disposed of as waste or used in low value applications, with significant negative economic and environmental impacts. This waste contains many highly valuable components, which if properly processed can be utilized to produce a range of high value products. For example, in Australian vegetable waste alone accounts for 277,000 tonnes of waste, which is 25% of total productionand again this primarily goes to landfill or is used as low value stock feed. The cost to growers is estimated at $155 million annually for the major vegetable crops.

In this presentation I will discuss projects examples where we are applying Green Chemistry principles for the conversion of biomass into bioproducts, with a focus on marine and agricultural underutilized biomass.

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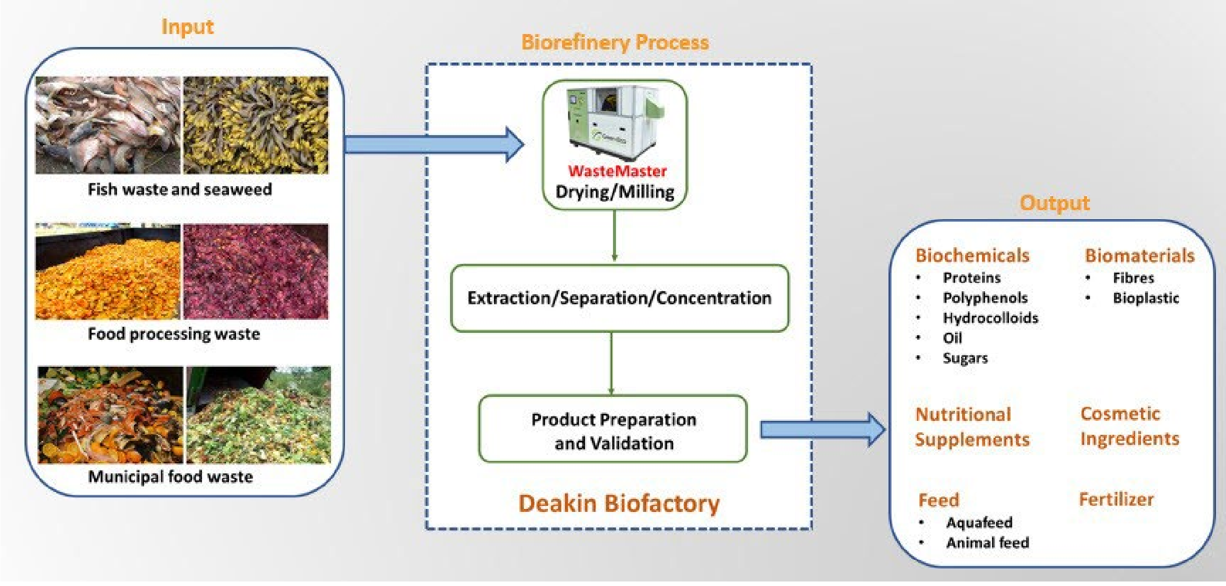

Figure: Bioprocessing to add value to underutilization biomass

ORAL SESSION 2, LECTURE THEATRE 401-401, 29 NOVEMBER, 2023, 4.40 – 4.55 PM

Extraction and Derivatisation of Hemicellulose for Novel Applications

Antonio F. Patti[1,2], Debjani Ghosh[1], Joanne Tanner[34] Gil Garnier[3,4]

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Hemicellulose is the third most abundant biomass component after cellulose and lignin. Depending on the biomass source, hemicellulose composition can vary from 20–35% by drymass in woods and other plants[1]. Hemicellulose is already an important source of commercially produced high-valued chemicals including xylose and xylitol[2].

In this study, an alkali mediated hydrothermal approach was optimised for partial extractionof high-purity hemicellulose (xylan) from a timber waste product (unbleached eucalyptus sawdust)[3,4]. The purified hemicellulose xylan was subsequently functionalised for potential new applications. A new class of multi stimuli-responsive hydrogel was developed in a one-step process, with an epoxide of 7-hydroxycoumarin. These novel hydrogels are UV stable with excellent UV protection properties, and are thus promising sustainable materials for applications in personal care, biotechnology and agriculture.

A second novel functionalisation was achieved by using the xylan as a carbohydrate donor, and glycerol carbonate was used as glycerol donor in a single step synthesis to produce dihydroxypropyl xylan. Glycerol modified sugars are naturally hydrating molecules of interest that can be explored as high-performance commodities and in applications for biomedical materials.

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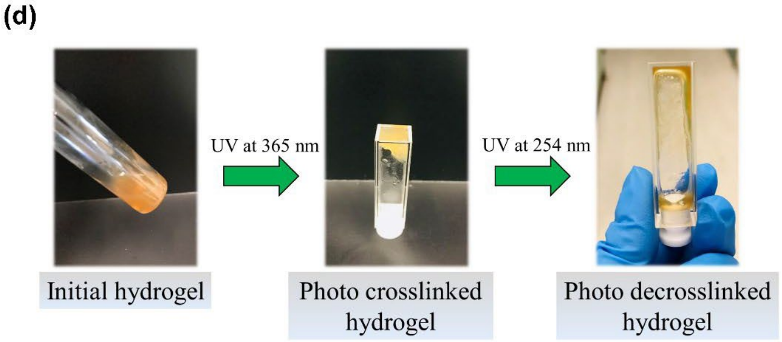

Figure 1

ORAL SESSION 2, LECTURE THEATRE 401-401, 29 NOVEMBER, 2023, 4.55 – 5.10 PM

Psidium guajava (Guava) leaves ash: A green heterogeneous catalyst for efficient biodiesel production

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In this work, we report the fabrication of highly porous basic heterogeneous catalyst from *Psidium guajava* leaves also commonly known as Guava leaves and its utilization in biodieselproduction. Series of catalyst were generated by calcinating dried and powdered leaves at variable temperatures viz. 550°C, 650°C, 750°C, 850°C and 950°C and the efficiency of each of these was evaluated. Characterization techniques like FT-IR, PXRD, TGA, SEM, EDS, TEM, XRF, BET, CO_2-TPD and XPS were performed to get information about the functionality, morphology and elemental properties of the catalyst. The influence of reaction parameters like oil to methanol ratio, catalyst loading, temperature, time and cosolvent loading on biodiesel yield was studied. Optimum yield of 95.8% was achieved in presence of catalyst fabricated at 850°C (GL-850) at room temperature when the reaction was performed for 3hrs with 1:17 oil to methanol ratio, 6wt% loading of catalyst and 15% loading of n-hexane as cosolvent. The product biodiesel was analyzed by ^{1}H-NMR and GC-MS. Recyclability test of the best catalyst (GL-850) was performed and it showed excellent result of 92.1% yield at the end of 5th cycle.The thorough characterization of the catalyst showed that the presence of elements like calcium (Ca) and potassium (K) were responsible for the basic nature of the catalyst thereby making it highly efficient for biodiesel production.

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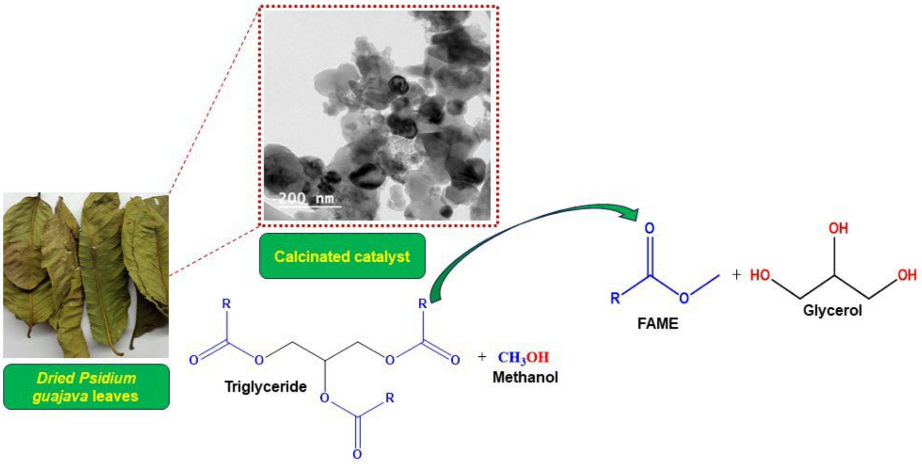

Figure: *Graphical abstract*

ORAL SESSION 2, LECTURE THEATRE 401-401, 29 NOVEMBER, 2023, 5.10 – 5.25 PM

Thermally insulating foams based on upcycled aramid nanofibers and nanocellulose

Lennart Bergström, Carina Schiele, Ehsan Hadi, Andi Di

Department of Materials and Environmental Chemistry, Stockholm University, Sweden

The production of textiles consumes a large amount of water and is responsible for large emissions of greenhouse gases. More than 80% of the textile fibres used for clothing are either burnt or disposed of in landfills, and recycling of used clothing is very small. Thermal insulation materials are essential to ensure and maintain a pleasant indoor climate in buildings. The most commonly used insulation materials are fossil-based and the energy needed to heat or cool buildings is directly related to thermal conductivity. Thermally superinsulating foams based on upcycled and biobased fibres could both significantly reducethe energy demand and carbon footprint, and promote the use of waste and renewable materials in the building sector. In this work, we will demonstrate how Kevlar® yarn can be upcycled into very thin and branched aramid nanofibers by a combination of chemical splitting and hydrothermal acid treatment ($upANF_A$). Light-weight hybrid foams of $upANF_A$ together with TEMPO-oxidized cellulose nanofibril (CNF) were prepared by ice-templating with highly aligned fibrils. The hybrid foams displayed a thermal conductivity below the value for air perpendicular to the aligned nanofibrils over a wide relative humidity range. The decrease of the thermal conductivity of the hybrid $upANF_A$/CNF foams with increasing $upANF_A$ content will be discussed and related to estimates of the phonon scattering at the CNF-$upANF_A$ interfaces. This work demonstrates how upcycled and renewable nanofibers with a small diameter can be integrated into super-insulating foams and illustrates how phonon scattering can be interfacially engineered.

ORAL SESSION 2, LECTURE THEATRE 401-401, 29 NOVEMBER, 2023, 5.25 – 5.40 PM

Hydrophobic pine bark extracts for the surface treatment of natural fibres

Regis Risani,[1] Maxime Nourtier,[1,2] Claire Mayer-Laigle,[1,3] Lloyd Donaldson,[1] Rachel Murray,[1] Marie-Joo LeGuen,[1] Stefan Hill[1], Robert Abbel[1]

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Bark is a heavily underutilised natural resource. In New Zealand, the forestry sector alone produces approximately 2.3 million metric tonnes of bark per year as a waste stream of wood production. The overwhelming majority derives from radiata pine which is the dominant tree in New Zealand's commercial forests. The Bark Biorefinery programme aims at unlocking this vast potential through the extraction of biobased components from pine bark and the identification of potential future uses. One exemplary application is the surface treatment of natural fibres with hydrophobic bark extracts (waxes) to improve their compatibility with biopolymers for the next generation of sustainable high-performance composites.[1]

In this work, super-critical CO_2 extraction was used to obtain hydrophobic waxes consisting mainly of long-chain fatty acids and alcohols. We have formulated these waxes into aqueousemulsions suitable for spray coating onto technical hemp fibres using the Maxi blender process.[2]

Successful coating of waxes on the fibres has been demonstrated and quantified through FTIR and NMR spectroscopies and fluorescence microscopy. We have also studied the thermal properties of the treated fibres which showed that they were sufficiently stable towithstand the processing temperatures during composite preparation. Through compounding with the biopolymer poly(butyl succinate), fibre-reinforced composites were produced.

Mechanical testing revealed only minor differences between the materials containing untreated and wax-coated fibres. These results suggest that the wax coatings had partially diffused into the biopolymer matrix. We are currently working on strategies to achieve a stronger binding between the waxes and the fibre surfaces.

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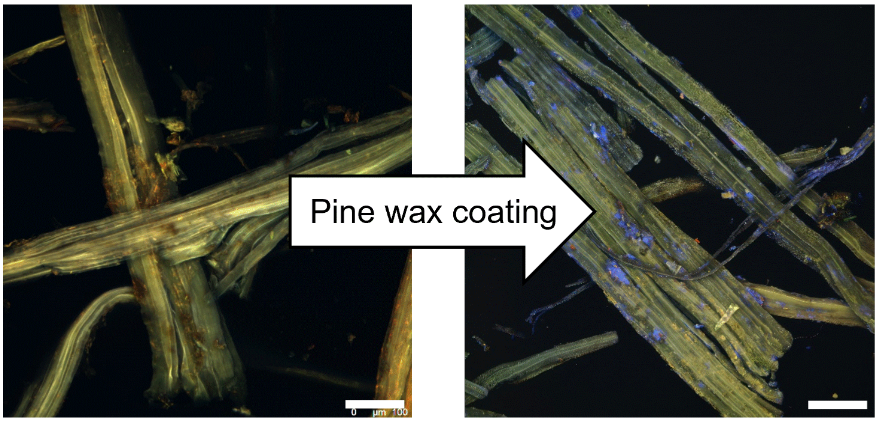

Figure: *Fluorescence microscopy images of hemp fibres prior to (left) and after (right) coating withpine wax extracts (blue). The scale bar corresponds to 100 micrometres.*

ORAL SESSION 2, LECTURE THEATRE 401-401, 29 NOVEMBER, 2023, 5.40 – 5.55PM

Eco-friendly recovery of alginate, fucoidan, and phenolics via aqueous ball milling of brown seaweed

Sachin Talekar[1,2] and Colin Barrow[1,2]

[1]*School of Life and Environmental Sciences, Deakin University, Waurn Ponds, Victoria 3216,Australia*

[2]*ARC Industrial Transformation Training Centre for Green Chemistry in Manufacturing*

The commercial production of brown seaweed phenolics and polysaccharides involves the energy-intensive drying of seaweeds followed by conventional extraction with organic solvents, acid, and alkali. Organic solvents used to extract phenolics are flammable and sometimes toxic [1]. Furthermore, acid and alkali used for polysaccharide extraction necessitate special equipment that is resistant to acidic and alkaline pH and generate a large amount of acidic and alkaline waste that must be treated before disposal [2]. Therefore, a green process based on aqueous ball milling of undried brown seaweed for the extraction of phenolics and polysaccharides (alginate and fucoidan) without the use of organic solvents, acids, or alkalis wasproposed (Figure 1). The ball milling treatment was optimized, and the maximum recovery of alginate (35.3-38.9%) and fucoidan (7.3-8.6%) were obtained with co-recovery of phenolics (2- 3%) by ball milling at 300 rpm for 3 hours with a liquid-solid ratio of 40. These product recoveries were comparable to those obtained through conventional extraction. The recovered alginate andfucoidan were chemically similar to commercial alginate and fucoidan as determined by IR and ^{1}H NMR, and they had molecular weights of 600-800 kDa and 8-10 kDa, respectively, and polydispersity of 1.8-1.9 and 1.1-1.2, respectively. The recovered fucoidan had higher sulphate content and antioxidant activity than conventional acid-extracted fucoidan, while phenolics had antioxidant activity comparable to conventional ethanol-extracted phenolics. These findings suggest that the proposed aqueous ball mill-based extraction process could have a significant impact on seaweed processing industry in terms of cost and sustainability.

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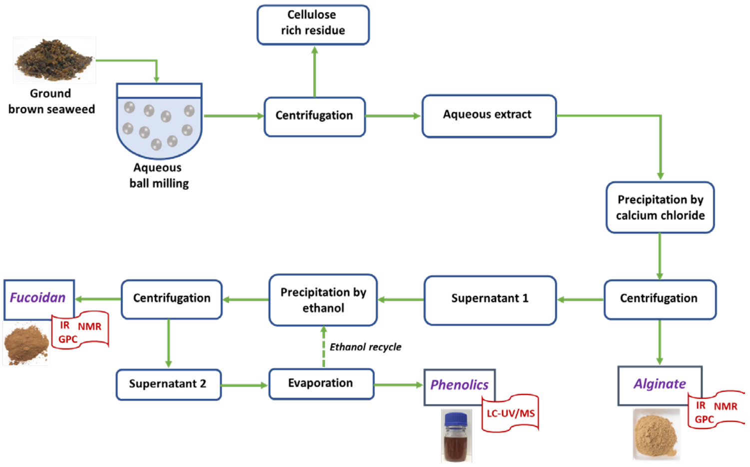

Figure. 1 Schematic illustration of the recovery of alginate, fucoidan, and phenolics using aqueous ballmilling of brown seaweed.

ORAL SESSION 2, LECTURE THEATRE 401-439, 29 NOVEMBER, 2023, 4.00 – 4.20 PM

Toward Greener Synthetic Routes to Gold and Silver Nanomaterials

Michelle D. Regulacio[1]

[1]*Institute of Chemistry, University of the Philippines Diliman*

Figure: Green-synthesized Au and Ag nanomaterials as SERS substrate and textile colorant.

Metal nanomaterials are attracting considerable research attention due to their numerous potential technological applications in a wide range of fields. In the case of strongly plasmonic metals, gold (Au) and silver (Ag), their nanostructured forms show great promise in SERS, catalysis, biomedicine, and textile functionalization. These nanomaterials are commonly prepared via wet-chemical methods using a variety of chemical reagents, each serving specific functions in the formation process. However, many of the reagents that are typically employed are toxic, expensive, and difficult to handle.[1] Our research focuses on developing green and facile synthetic methodologies for the preparation of Au and Ag nanomaterials using environmentally compatible and low-cost natural antioxidants as key reagents.[2] The reaction can be carried out at low temperature conditions, and water can be conveniently used as the solvent. Additionally, this antioxidant-mediated approach can be readily accomplished through simple benchtop experiments without requiring complex experimental laboratory set-ups. The green-synthesized Au and Ag nanomaterials can be potentially used as SERS substrates for detection of pollutant dyes and as textile colorants. In exploring greener methodologies of producing valuable metal nanomaterials, we are taking significant strides on the path toward clean and sustainable technologies.

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ORAL SESSION 2, LECTURE THEATRE 401-439, 29 NOVEMBER, 2023, 4.20 – 4.40 PM

Precisely controlled single atom and nanocluster-based materials: from fundamentals to applications in catalysis and energy

Vladimir Golovko,[1,2] Shailendra Sharma,[1,2] Johan Hammonet,[2,3] Hanieh Mousavi,[4] Sally Brooker,[2,5] Gregory Metha,[4] Aaron Marshall,[2,3]

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This talk will highlight an interesting approach towards fabrication of atomically precise catalytically active sites based on a single atom sites of metal clusters with specific number of metal atoms per cluster core (Figure). Unique nature of the metal clusters and earlier catalytic studies by our team will be highlighted first.[1-13] The most recent examples of catalytic studies in electrocatalytic hydrogen production and carbon dioxide conversion to more chemically useful carbon monoxide will be highlighted in the main part of this talk along with detailed characterisation of the catalytically active materials.[14-19]

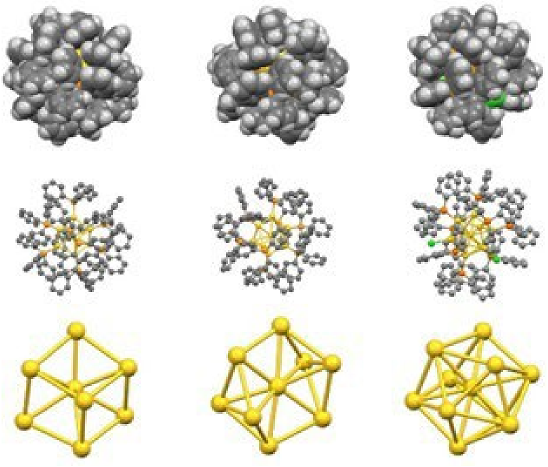

Figure: *Structures of selected gold clusters. Left – Au_8, middle – Au_9, right – Au_{11}. Top – spacefill model, middle – ball and stick model, bottom – magnified metal cores of the clustershighlighting atomic precision of these species*

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ORAL SESSION 2, LECTURE THEATRE 401-439, 29 NOVEMBER, 2023, 4.40 – 4.55 PM

Development of metal nanoparticle catalysts modified using multidentate polyoxometalates

Kang Xia,[1] Takafumi Yatabe,[1] Kentaro Yonesato,[1] Tomohiro, Yabe,[1] Kosuke Suzuki,[1] Kazuya Yamaguchi.[1]

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Gold nanoparticles have unique physiochemical properties, making them a subject of great interest as catalysts. Recently, theoretical studies reveal that “anionic” gold nanoparticles can effectively activate molecular oxygen (O_2) for oxidation reactions using O_2 as the sole oxidant.[1] However, due to the complexity and difficulty of designing these catalysts, limited studies have been reported.[2] Herein, we report a feasible methodology of obtaining stable and reactive “anionic” gold nanoparticle catalysts by utilizing multidentate polyoxometalates (POMs) as protecting ligands toward efficient oxidation reactions using O_2 as a greenoxidant.[3] We confirmed the existence of robust electronic interaction between gold nanoparticles and multidentate POMs, and the electronic states and reactivity of the gold nanoparticle catalysts can be sequentially modulated (**Figure 1a**). Notably, these catalysts (e.g. Au-**SiW9**/C) display excellent performance in oxidative dehydrogenation of piperidone derivatives to the corresponding enaminone products. Furthermore, these catalysts possessed higher stability than conventional gold nanoparticle catalysts without this modification (e.g. Au/C, **Figure 1b**). Our findings highlight the ability of inorganic multidentate POM ligands, bearing structural stability, steric and electronic effect, to confer long-lived and highly reactive characteristics upon gold nanoparticles. These approaches can be further extended to preparing various metal nanoparticles other than gold, enabling the design of novel nanomaterials for the development of environmentally benign reactions.

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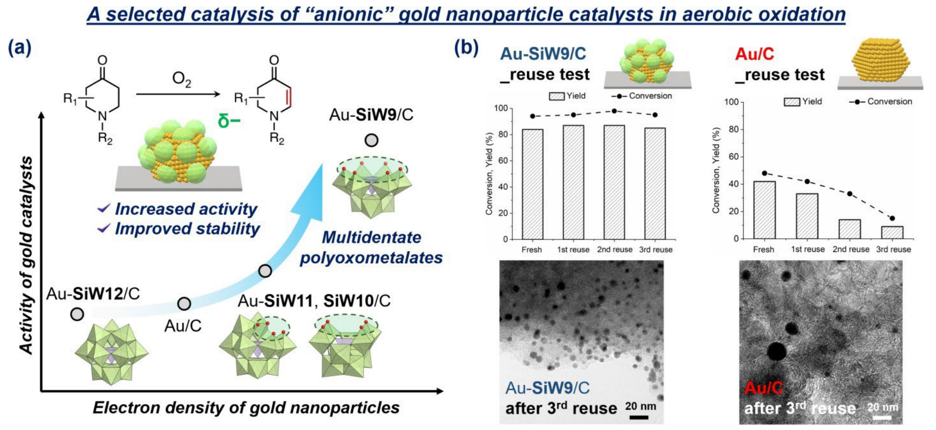

***Figure 1**: Anionic gold nanoparticle catalysts modified using multidentate POMs.*

ORAL SESSION 2, LECTURE THEATRE 401-439, 29 NOVEMBER, 2023, 4.55 – 5.10 PM

Development of High Entropy Alloy Subnanocluster Catalysts and its Structural Reversibility under Oxidative/reductive Conditions

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High entropy alloys (HEAs) have been attracted much attention in various fields due to their unique properties originating from the high configurational entropy. In this study, the sub- nanometric HEA clusters were successfully synthesized by utilizing the hydrogen spillover on CeO_2 nanorods (NRs). Additionally, the sub-nanometric HEA clusters demonstrated the reversible structural transformation under oxidative NO condition and reductive H_2 condition[1]. To synthesize the CoNiCuZnPd clusters supported on CeO_2-NRs (CoNiCuZnPd/CeO_2-NRs), Co^{2+}, Ni^{2+}, Cu^{2+}, Zn^{2+}, and Pd^{2+} were deposited on CeO_2-NRs by simple impregnation methods. Subsequently the specimen was reduced by H_2 at 600 °C to yield CoNiCuZnPd/CeO_2-NRs. The EDX mappings of CoNiCuZnPd/CeO_2-NRs indicated the formation of small HEA clusters. The coordination number (CN) of metallic bonds were determined to be 5.6 by the curve fitting of FT-EXAFS, which indicate that the diameter of clusters is 0.79 nm. The catalytic activity of HEA clusters was assessed by the NO reduction by H_2. The CoNiCuZnPd/CeO_2-NRs exhibited higher activity in comparison with monometallic Pd/CeO_2-NR catalyst (Fig. 1(a)). Additionally, the stability of HEA catalystswas evaluated by *in situ* XAFS under NO/H_2 conditions. In the case of quinary CoNiCuZnPd/CeO_2-NRs, the randomly distributed Pd atoms formed core nuclei encapsulated by non-noble metal oxide shells (Pd@MO_x) via the sacrificial oxidation of the base metals under NO. atmosphere These structures could be reversibly changed back to well-mixed HEA nanoclusters under a H_2 atmosphere (Fig. 1(b)).

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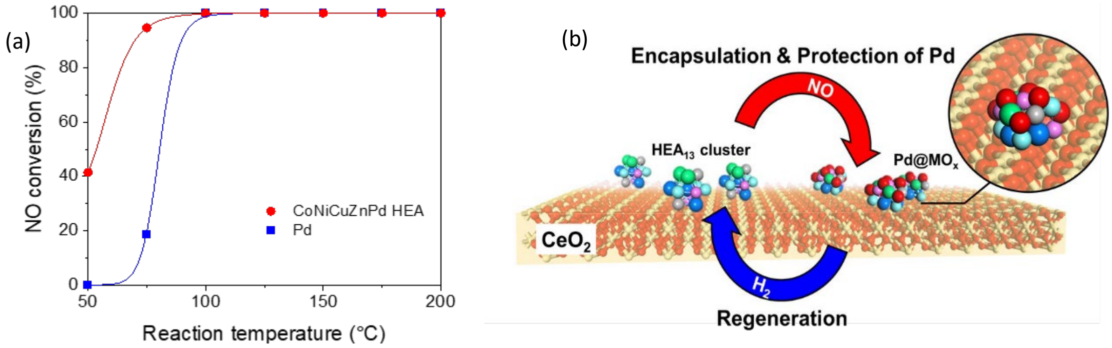

Figure 1 *(a) NO reduction activity of CoNiCuZnPd/CeO_2-NRs and Pd/CeO_2-NRs. (b) Proposed structural changes of CoNiCuZnPd/CeO_2-NRs under NO/H_2 conditions.*

ORAL SESSION 2, LECTURE THEATRE 401-439, 29 NOVEMBER, 2023, 5.10 – 5.25 PM

Atomically Dispersed Co-Ni Dual-Metal Sites Showing Unique Reactivity and Dynamics for the Oxygen Evolution Reaction

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Understanding the structural evolution of electrocatalysts under working conditions is vital foroptimizing performance, especially for oxygen evolution reaction (OER), a key process in water splitting. Herein, we demonstrate that the pyrolysis of Co/Ni-doped MAF-4/ZIF-8 yields porous nitrogen-doped carbons functionalized with atomically dispersed Co-Ni dual-metal sites possessing an unprecedented N8V4 structure (where N denotes the total number of nitrogen atoms bonding the two metals and V denotes the number of missing carbon atoms).The dual-metal sites enabled a unique hydrogen-bonding promoted mechanism for OER in alkaline media, involving the *in situ* oxidation of the carbon support adjacent to the metal sites to form C-OH groups. Density functional theory calculations demonstrate that the flexible C-OH groups can form reversible hydrogen bonds with the OER intermediates, thereby boosting OER kinetics by breaking the conventional scaling relationships between the elementary reactions in the $4e^-$/$4H^+$ oxidation process.

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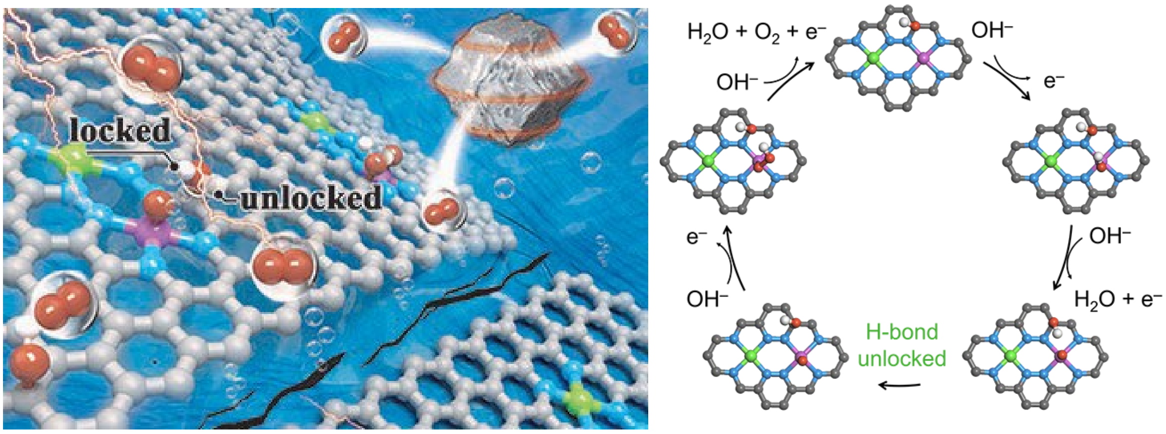

Figure: *(left) Schematic showing N8V4-CoNi dual-metal sites on N-doped carbons, which cause in situ oxidation of the N-doped carbon substrate for enhanced OER performance. (right) Proposed OER mechanism for N8V4-CoNi-OH sites.*

PLENARY SESSION 2, LECTURE THEATRE 401-401, 30 NOVEMBER, 2023, 9.00 – 10.00 AM

Harnessing AI for Green and Sustainable Chemistry towards Carbon Neutrality

Xiaonan Wang[1, 2]

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[2]*Department of Chemical and Biomolecular Engineering, National University of Singapore,Singapore*

The rapid evolution of Artificial Intelligence (AI) offers enormous opportunities for the realm of green and sustainable chemistry. Data-driven strategies are transforming traditional research paradigms that often reply on exhaustive trial-and-error approaches. As the global emphasis intensifies on carbon neutrality, AI emerges as a pivotal tool to navigate the complexities of sustainable chemical innovation.

This talk will shed light on how AI, especially machine learning (ML), can redefine traditional workflow, streamlining the discovery and design processes inherent in green chemistry. These AI methods facilitate a deeper understanding of sustainable chemical processes, ensuring reduced waste, enhanced resource efficiency, and the identification of environmentally benign alternatives. The integration of machine learning in the loop via active learning strategies expedites the discovery of environmentally benign catalysts, membranes, renewable energy materials, and waste-minimizing solutions. By introducing an AI-integrated multi-scale chemical data platform, we demonstrate the integration of high-throughput computational and experimental methods with sustainable chemical preparation and characterization techniques. Such integration has proven instrumental in pioneering carbon-neutral technologies, highlighting innovations in eco-friendly catalysts, sustainable membrane materials, and next-generation energy solutions. Moreover, the inherent capability of AI to adeptly guide experiments, coupled with its vast data processing abilities, augments our understanding of the expansive design space.

In conclusion, this talk will provide insights into the future landscape of AI-enhanced green and sustainable chemistry, underscoring the promises, potential applications, and the inevitable challenges. The synergy of AI and green and sustainable chemistry will be more and more promising with broader community efforts in building open database and platforms.

KEYNOTE SESSION 2, LECTURE THEATRE 401-401, 30 NOVEMBER, 2023, 10.00 – 10.30 AM

Self-healing polymers from biobased compounds

Kei Saito

Graduate School of Advanced Integrated Studies in Human SurvivabilityKyoto University, 606-8306, Japan

Traditionally, polymers have been designed to possess irreversible covalent bonds between the repeating monomer units. However more recently, significant interest has been directed toward the synthesis of dynamic polymers that are held together by dynamic (reversible) covalent or non-covalent bonds which can be used as self-healing materials. This study focused on the production of the novel self-healing materials from lignin. Glycerol-derived polyfunctional monomers having cinnamate groups were produced using a sustainable process from vanillin and syringaldehyde, two compounds readily obtained from the oxidation of lignin to synthesize bio-based photo-crosslinkable/decrosslinkable self-healing polymers. Other types of self-healing polymers from biobased compounds such as soybeanoil will also be presented.

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ORAL SESSION 3, LECTURE THEATRE 401-401, 30 NOVEMBER, 2023, 11.00 – 11.20 AM

CO2-derived oxalic acid-assisted conversion of organic and inorganic resources

Shinji Kudo,[1]

[1]*Institute for Materials Chemistry and Engineering, Kyushu University, 6-1, Kasuga Koen,Kasuga, 816-8580, Japan*

This presentation will introduce our on-going two research projects related to carbon recycling technology. The projects propose processes for the conversion of inorganic (iron ore) and organic (lignocellulosic biomass) resources with CO$_2$-derived oxalic acid as a key compound. The first process[1] enables, utilizing characteristics of oxalic acid and its salts, lowtemperature production of high-purity metallic iron from a variety of iron ores. The second process aims to produce platform chemicals, including biomass-derived levoglucosenone and oxalic acid, along with their derivative biopolymers using CO$_2$ as feedstock and syntheticagents. The presentation will cover the current progress of the projects, and the challenges that need to be addressed.

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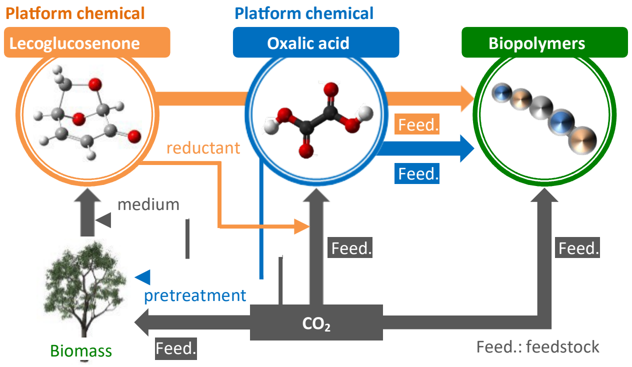

Figure: CO$_2$-assisted production of platform chemicals and biopolymers from lignocellulosic biomass(organic resource)

ORAL SESSION 3, LECTURE THEATRE 401-401, 30 NOVEMBER, 2023, 11.20 – 11.40 AM

Computational prediction of the catalyst surface hydrogen coverage in the hydrogenolysis of plastic waste

Martina Lessio,[1] Fabio Colasuonno,[1] Michele Pettini,[1] Sohaib Umer,[1]

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Catalytic hydrogenolysis on supported metal nanoparticles has recently emerged as a promising technique for the conversion of polyolefin-based plastic waste into useful productsunder moderate conditions.[1,2] However, more control over the product distribution is needed in order for this process to be employable at the industrial scale. Fundamental mechanistic insights are critical to achieve such control, with computational methods being the ideal tool to gain these insights. In this contribution, I will present our recent work on ruthenium- catalysed hydrogenolysis of polyolefin-based plastic waste. In this work, we use dispersion- corrected density functional theory (DFT) to accurately determine the surface coverage of atomic hydrogen under operating conditions; this parameter is known to significantly influence reaction outcomes and selectivity. Specifically, we show that the approach typically used in the literature for this purpose fails to correctly predict the results of existing scanning tunnelling microscopy experiments. We thus establish a different protocol that successfully reproduces these data and can be used to accurately assess the surface coverage under catalytic conditions. We then use this protocol to study the atomic hydrogen coverage on different ruthenium surfaces with the aim of predicting their different activity andselectivity.

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ORAL SESSION 3, LECTURE THEATRE 401-401, 30 NOVEMBER, 2023, 11.40 – 11.55 AM

Waste Plastics as Resources for Functional Material and Chemical Production

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More than 300 million tonnes of petroleum-based plastics are produced annually to meet their ubiquitous demands in all aspects of modern life. However, most plastics have very unsustainable take-make-throw life cycles, with only a small fraction being recycled yearly. As such, there has been increased attention to give these end-of-life plastics new life as societally-relevant functional polymeric materials and industrially-viable small molecule chemicals.[1] In this presentation (Figure 1), we discuss some of our recent efforts to increase the range of possible materials accessible from the most common waste plastics. These include our efforts to valorise waste plastics PET into polymer electrolytes that can be assembled into working lithium ion battery prototypes, as well as transformation of PE into water-soluble antifungal polymers with efficacy against pathogenic *Candida* fungi. In addition, our recent successes in sustainable metal-free oxidative degradation of waste polystyrene using O_2 into industrially-valuable aromatic acids, whose global demand exceeds 500,000 tonnes annually, will be presented. The presentation will end with a discussion of further possibilities of upcycling every class of the most common waste plastics today. The exploitation of high-volume waste plastics as a feedstock for production of such diverse products highlight the potential of this emerging approach in waste plastic valorisation, simultaneously contributing towards the creation of a more sustainable future materials economy.

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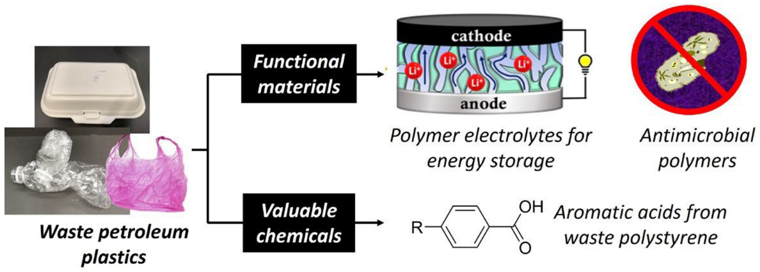

Figure 1: Valorisation of waste petroleum plastics into polymer electrolytes, antimicrobial compounds and industrially-relevant organic acids.

ORAL SESSION 3, LECTURE THEATRE 401-401, 30 NOVEMBER, 2023, 11.55 AM – 12.10 PM

Fluorous Nanochannels Enabling Ultrafast Desalination

Shuo Chen[1], Yoshimitsu Itoh[1,2], Ryota Hirahara[1], Takeshi Konda[1], Tsubasa Aoki[1], Kohei Sato[1], and Takuzo Aida[1,3]

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[2]*JST-PRESTO*

[3]*RIKEN CEMS*

Desalination is a crucial technology for producing potable water from seawater. While the hydrophobic interior surface of water channel protein aquaporins has been recognized for its role in efficient desalination[1], the potential of nanochannels with a fluorinated superhydrophobic interior surface remains unexplored. Recent findings indicate that water clusters in the vicinity of fluorinated compounds break apart, resulting in the generation of hydroxy dangling bonds, whereas hydrocarbon analogues produce significantly fewer dangling bonds[2,3]. This observation suggests that nanochannels with a fluorinated interior surface may suppress the formation of water clusters, which are likely to diffuse more slowly than individual water molecules. The objective of this study was to investigate desalination through fluorous nanochannels.

In this research, we present a series of fluorous oligoamide macrocycles with varying interior diameters, capable of undergoing supramolecular polymerization within phospholipid bilayer membranes to form fluorous nanochannels[4]. The nanochannel with an inner diameterof 0.9 nm exhibited a water permeability two orders of magnitude higher than that of aquaporins or carbon nanotubes, which are usually regarded as efficient water channels. Moreover, the electronegativity of the fluorous interior contributes to near-perfect salt reflectance, enhancing its potential for desalination applications.

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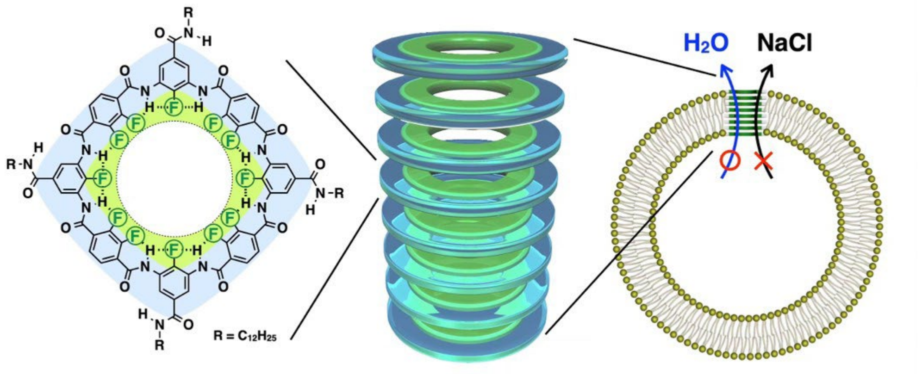

Figure: A representative fluorous nanochannel for ultrafast desalination

ORAL SESSION 3, LECTURE THEATRE 401-401, 30 NOVEMBER, 2023, 12.10 – 12.25 PM

Evaluation of the microbial hydrogenotrophic methanation process for power to gas

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[2]*Clean-Energy Research Institute, Hanyang University, Seoul, Korea*

Microbial hydrogenotrophic methanation using autotrophic methanogens could be operated at relatively low temperatures and pressure, which is easier than the conventional chemical methanation processes. In power-to-gas systems, hydrogenotrophic methanogens use CO_2/H_2 as the sole carbon and energy source for methane production. The gas-liquid mass transfer of H_2 is a crucial factor controlling the efficiency of the biological methanation process. Improving the solubility of hydrogen with a low henry's law constant is still in the-state-of-the-art for better system efficiency and requires more research. A 2400 L pilot scale reactor comprised of a continuously stirred tank and three pithed blade-type impellers was used to get a high H_2 mass transfer. The reactor was operated for a biological methanation process using a thermophilic hydrogenotrophic methanogen, *Methanothermobacter sp.* KEPCO-2. In the newly designed reactor, the conversion efficiencies of CO_2 and H_2 reached 97.1% and 97.9%, respectively and the maximum methane production rate was observed about 400 VVD (L/L/d). The high-purity methane from the reactor can be connected to the gas grid without additional processing stages.

ORAL SESSION 3, LECTURE THEATRE 401-439, 30 NOVEMBER, 2023, 11.00 – 11.20 AM

Quantifying reaction outcomes in ionic liquids

Jason B. Harper,[1,3] Maxwell D. Coney,[1] Kofoworola Gbayo,[1] Alyssa Gilbert,[1] Andrew Y. Hsieh,[1] Daniel C. Morris,[1,2,3] Ronald S. Haines,[1] Stuart W. Prescott[2] and William S. Price[3]

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Ionic liquids have been suggested as replacements for organic solvents in preparative chemistry since their emergence at the end of the last century.[1] However, changes in reaction outcome relative to molecular solvents[2] have limited their application.

Our group has focused on understanding these ionic liquid solvent effects, with microscopic interactions interactions in solution being able to explain how solvent effects vary with the amount and nature of the ionic liquid.[3] Such understanding has allowed solvent design to control reaction outcomes[4] and has allowed us to diversify into structural studies in these systems and how they affect reaction outcomes.[5]

Lacking at this stage is the ability to quantitatively predict these solvent effects. While the existing predictive framework can identify the optimum proportion of the best ionic liquid(s) to affect reaction outcome, whether this results in a change in (say) rate constant of two- or ten-fold remains elusive. This presentation will introduce a range of questionably successful solvent parameters, introduce the possibility for machine learning approaches of various styles,[6] identify that structural features might correlate to reactivity[7] but that, ultimately, resorting to formal physical organic reactivity parameters[8] does the trick (Figure 1).[9]

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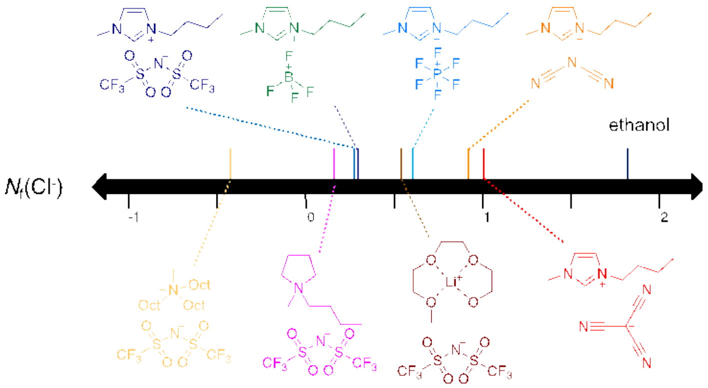

Figure 1. The nucleofugality (leaving group ability) of chloride in ionic liquids ($\square_{IL}$ = 0.8 in ethanol).[9]

ORAL SESSION 3, LECTURE THEATRE 401-439, 30 NOVEMBER, 2023, 11.20 – 11.40 AM

Amphiphilic Ionic Liquid cytotoxicity: structure-activity and mechanistic studies

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Ionic liquids (ILs) were considered to be environmentally friendly and safe alternatives to conventional solvents, however accumulating evidence suggests that some ILs, particularlyamphiphilic ILs (AmILs), are cytotoxic towards a variety of organisms. Given their high aqueous solubility and chemical stability, cytotoxic ILs have the potential to become significant environmental pollutants similar to perfluoroalkyl substances.[1] It is therefore important to understand the mechanism and the structural features associated with IL cytotoxicity, and this presentation will discuss our work in this area.

Previous mechanistic studies suggested that AmILs either disrupt cell membranes or induce mitochondrial dysfunction to trigger cell death.[2] Structurally related triphenylphosphonium cations are known to accumulate in mitochondria in response to the membrane potential across the inner mitochondrial membrane (IMM), and we hypothesised that AmILs would show similar subcellular localisation. Using confocal microscopy we show that a fluorescent AmIL rapidly accumulates in cell mitochondria, and that AmILs produce a series of effects that are consistent with permeabilisation of the IMM.[3] These effects are associated with cell death, and establish the IMM as a likely target of cytotoxic AmILs.

We have also sought to expand the structure-activity relationship (SAR) for IL cytotoxicity by assessing the impact of cationic headgroup structure on cytotoxicity. Headgroup features including size, charge, and lipophilicity were examined, and changes in cytotoxicity were linked to the capacity of the AmILs to disrupt the IMM.

We hope these findings assist in the design of ILs with reduced cytotoxicity and potential to become environmental pollutants of concern.

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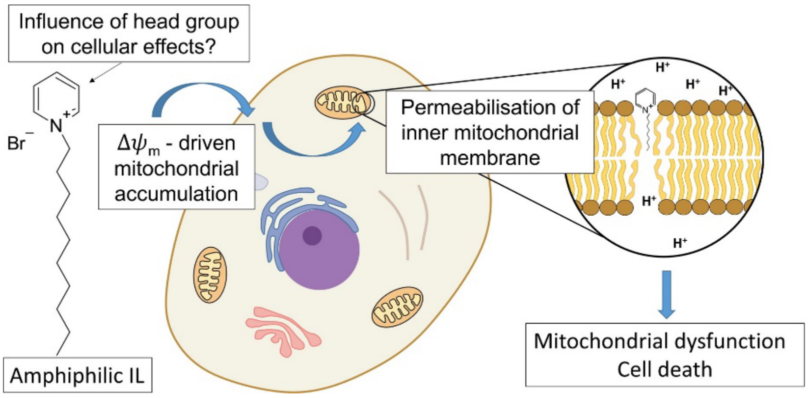

Figure: Proposed mechanism of IL induced cytotoxicity.

ORAL SESSION 3, LECTURE THEATRE 401-439, 30 NOVEMBER, 2023, 11.40 – 11.55 AM

Sub- and supercritical fluids for the biomass conversion

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Due to the pressing issue of global warming, there has been a significant focus on producingcarbon-neutral fuels and chemicals from renewable and sustainable resources. Sub- and supercritical fluid biomass conversion has garnered attention due to its advantageous physicochemical properties, including zero surface tension, fast reaction rates, deoxygenation ability, and the suppression of coke formation. This approach is seen as one of the most promising methods to effectively utilize technologically challenging feedstocks. This presentation is divided into two parts. The first part will explore the traditional hydrothermal and solvothermal liquefaction of various types of biomass, such as woods, microalgae, and sewage sludge [1–8]. Under supercritical ethanol conditions, complete conversion of biomass into liquids and gases has been achieved. During the liquefaction process, some fraction of ethanol reacts with the reactants and intermediates. By skillfully separating the products, higher bio-oil yields can be obtained, leading to improved process efficiency. In the second part of the talk, the focus will shift to solvent participation during the catalytic conversion of biomass constituents [9–14]. Over heterogeneous catalysts, waterand ethanol molecules donate their hydrogen to reactants, such as furfural, altering the reaction pathways. The influence of solvents on product selectivity will be discussed, offeringinsights into enhancing the overall conversion process.

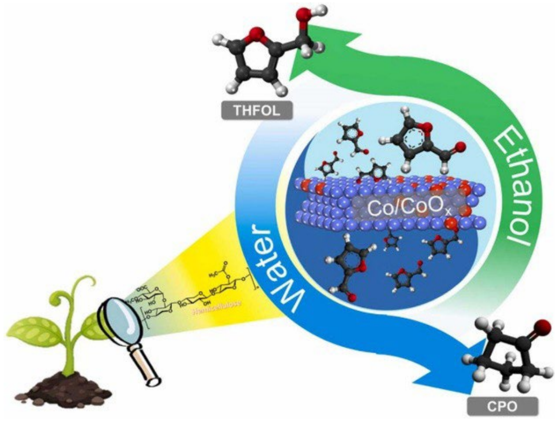

Figure 1: Solvent-mediated product control

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ORAL SESSION 3, LECTURE THEATRE 401-439, 30 NOVEMBER, 2023, 11.55 AM – 12.10 PM

Hydroxide-ion induced efficient mineralization of poly(vinylidene fluoride) and related copolymers in subcritical water

Hisao Hori,[1] Jin Hamaura,[1] Ryo Honma,[1] Abdelatif Manseri,[2] Bruno Ameduri[2]

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Fluoropolymers have been used in many industrial equipment because of their high stability against temperature, chemicals, ignition, and UV-light irradiation.[1] Among them, poly(vinylidene fluoride) (PVDF) and related VDF copolymers have combined characteristics of the high stability of fluorochemicals with the melt processability of thermoplastic polyolefins. Therefore, they have been used for chemical- and electrical processes and energy-related applications.[2] While usages of the fluoropolymers have spread, waste treatment techniques do not catch up with their increasing demand. Incineration is an option. However, HF gas generated during the treatment seriously damages the incinerators.

Therefore, most of the wastes are disposed of in landfill.[3] If fluorine atoms in the wastes are transformed into F^- ions by means of environmentally benign methodologies, the F^- ions canreact with $Ca(OH)_2$ to form CaF_2 as fluorspar mineral. Nowadays, the mine production of high-purity fluorspar, suitable for hydrofluoric acid production, is limited in a few countries. Because hydrofluoric acid is a raw material for all fluorochemicals, the development of an efficient decomposition technique of fluoropolymers to F^- ions would contribute toward closing the loop of fluorine element. This presentation shows an effective method for complete defluorination of PVDF and related copolymers to F^- ions, by means of subcriticalwater at relatively low temperature (250 °C) in the presence of an alkali reagent.[4] The formation of artificial fluorspar upon addition of $Ca(OH)_2$ to the resulting reaction solution is also reported.

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ORAL SESSION 3, LECTURE THEATRE 401-439, 30 NOVEMBER, 2023, 12.10 – 12.25 PM

Catalytic decomposition of polypropylene in petroleum-based solvents

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Focusing on chemical recycling, we aimed at developing a catalytic conversion process for waste plastics into petrochemical feedstocks. Waste plastics were dissolved in hydrocarbon solvent to improve fluidity and remove undesirable substances, and then converted to petrochemical feedstocks (C_5-C_9 products) by catalytic decomposition. Polypropylene (PP) was used as plastic and Beta zeolite as catalyst. Light Gas Oil (LGO) and Light Cycle Oil (LCO) were used as petroleum-based solvents (RBC-LGO, RBC-LCO) after removing basiccompounds by solid acid treatment[1]. The fraction of aliphatic hydrocarbons was high in RBC-LGO, while that of aromatic hydrocarbons was high in LCO. In addition, *n*-Cetane (*n*- C_{16}) and 1-Methylnaphthalene (1-MN) were used as solvent to represent linear alkane and aromatic hydrocarbon. The decomposition behavior of PP, e.g., the PP conversion, in such petroleum-based solvents was studied.

The decomposition tests were carried out using 20 g of solvent, 5 g of PP, and 1 g of Beta zeolite at 673 K for 60 min in the batch reactor. When RBC-LGO and RBC-LCO were usedas solvent, the PP conversion was 97.0% and 58.4%. When *n*-C_{16} and 1-MN were used assolvent, the PP conversion was 96.9% and 68.2% suggesting that aromatic hydrocarbon negatively influenced the PP conversion. Therefore, a solvent containing aliphatic hydrocarbon such as RBC-LGO was recommended for PP conversion.

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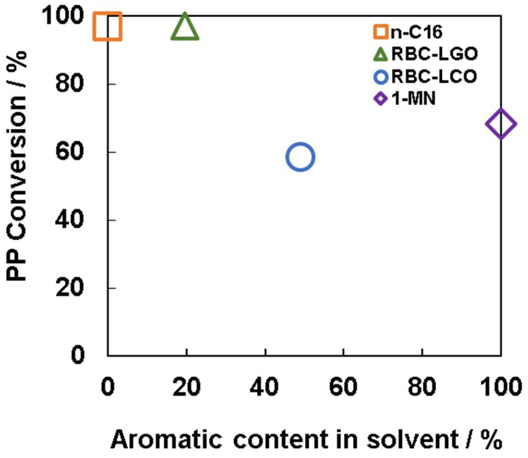

Figure 1: Relationship between aromatic content in solvent and PP conversion after 60 min at 673 K.

Acknowledgement This work was partially supported by NEDO Grant Number JPNP20012.

ORAL SESSION 4, LECTURE THEATRE 401-401, 30 NOVEMBER, 2023, 1.30 – 1.50 PM

Direct Conversion of Low-Concentration of CO2 to Polyurethane Raw-Materials Using an Organic Base as CO2 Capture Agent

Katsuhiko Takeuchi

National Institute of Advanced Industrial Science and Technology (AIST).

Conversion of CO_2 emitted from thermal power plants into basic chemicals is an effective way to reduce anthropogenic emissions of CO_2, which is considered a major cause of global warming. However, CO_2 in the exhaust gas emitted from thermal power plants is of low concentration and purity, and its purification, concentration, and compression require a great deal of energy and cost. Therefore, the direct utilization of CO_2 in the exhaust gas emitted from thermal power plants without such pre-treatment processes should be significant. In this presentation, we introduce the synthesis of carbamic acid esters (CAEs), which are useful raw materials for polyurethanes, from the model exhaust gas of thermal power plants using regenerable alkoxylating agents such as titanium and silicon alkoxides, and an organic strong base that can capture CO_2.[1,2] This method is environmentally friendly and economical for the production of polyurethane raw materials because it consumes practically only amines, alcohols, and CO_2, with only H_2O as a by-product.

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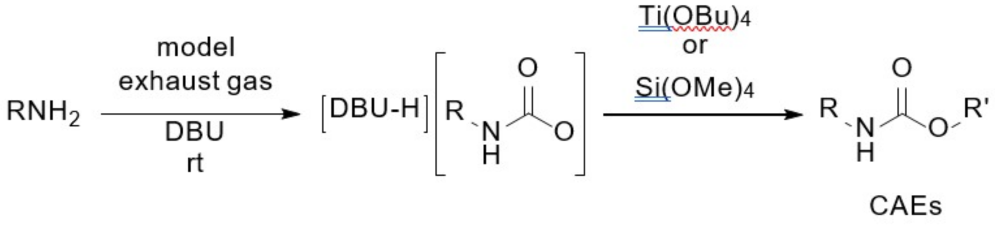

model exhaust gas: 15 vol% CO_2, 300 ppm of CO, 500 ppm of NO_2, 500 ppm of SO_2, balance N_2.

Figure: Direct synthesis of CAEs from CO_2 in model exhaust gas of the thermal power plant.

This work was supported by the Uncharted Territory Challenge 2050 from the New Energy and Industrial Technology Development Organization (NEDO).

ORAL SESSION 4, LECTURE THEATRE 401-401, 30 NOVEMBER, 2023, 1.50 – 2.10 PM

Multi-scale modeling of the electrochemical CO2 reduction reaction: Challenges and opportunities

Yu Mao[1]*, Ziyun Wang[1], and Geoffrey I.N. Waterhouse[1]

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The electrochemical CO_2 reduction reaction (CO_2RR) is expected to play a vital role in achieving carbon neutrality in the energy sector. While substantial progress has been made experimentally relating to electrocatalyst development for the CO_2RR, fundamental understanding the CO_2RR at a microscopic level is still lacking. Herein, starting with a simpleCu surface, we introduce models for simulating CO_2RR at different length and time scales. Utilizing some of the latest computational techniques (large-scale *ab initio* molecular dynamics, machine learning, constant potential method, *etc.*), we have successfully simulated the influence of water's hydrogen bonding network on the selectivity of CO_2RR (Fig. a), demonstrating that C_{2+} selectivity can be enhanced by tuning the hydrogen bond network of water in a nano-confined space [1]. In addition, on a larger scale, we used constant-potential molecular dynamics to study the impact of electrode potential, alkali metal ions (K^+), and organic polymers in a cationic-group-functionalized CO_2RR system (Fig. b) [2].Given its large size, this model can explore issues that traditional *ab initio* methods cannot, and successfully explains the impact of alkali metal cations (K^+) or cationic organic polymers on CO_2RR selectivity. By integrating algorithms at different scales (*e.g.,* density functional theory, classic molecular dynamics, finite element method, *etc.*), it should be possible to model different CO_2RR systems in a more accurate manner, paving the way towards rational catalyst design for CO_2 valorisation using renewable electricity.

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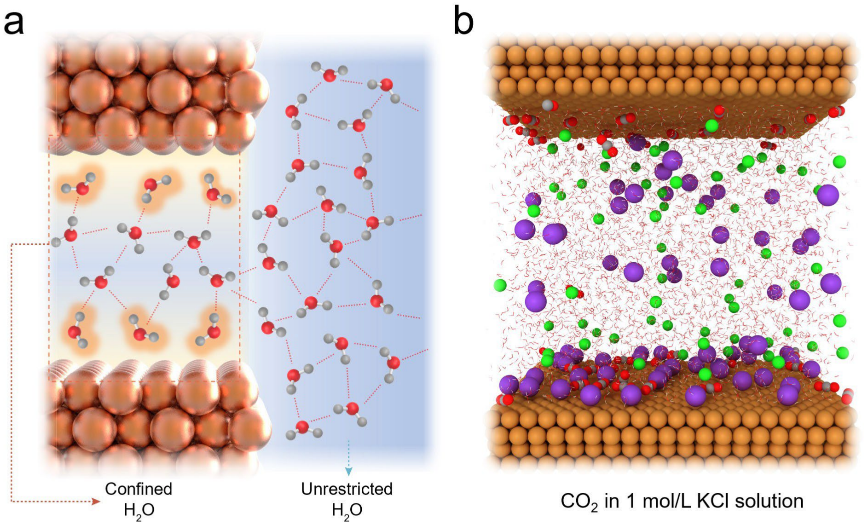

Figure: Structural models of **a** confined and unrestricted H_2O in a Cu nanocavity; **b** CO_2 in a 1 mol/L KCl solution between Cu electrodes. Purple, green, brown, and red balls represent K, Cl, Cu, and O,respectively.

ORAL SESSION 4, LECTURE THEATRE 401-401, 30 NOVEMBER, 2023, 2.10 – 2.25 PM

Methanol Production by CO2 Hydrogenation Catalyzed by Dinuclear Iridium Complexes under Gas-Solid Phase Conditions

Yuichiro Himeda,[1]

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Development of efficient CO_2 conversion to methanol as a useful chemical and fuel is intensively in progress.[1] However, conventional Cu-base catalysts which operated at above 200 °C suffers from low conversion and selectivity. Herein, we present catalytic hydrogenation of CO_2 to methanol using multinuclear iridium complexes in a gas–solid phase reaction under mild reaction conditions.[2]

In our previous study, we have reported that CO_2 hydrogenation in acidic aqueous solution at 70 °C provided mainly to formic acid (FA) along with a small amount of methanol even under high pressure conditions.[3] From these results, we concluded that the equilibrium limitation between FA and CO_2/H_2 in water suppresses further hydrogenation of FA to methanol. In order to circumvent the equilibrium limitation, we envisioned novel approach formethanol production using dinuclear iridium complex **2** under gas-solid phase conditions. Toour delight, when the reaction was performed using dinuclear iridium complex **2**, methanol was produced with high selectivity under mild reaction conditions (Table). On the other hand,using mononuclear analog **1** produced a negligible amount of methanol. It is worth noting that methanol was generated catalytically, even at low pressure and low temperature(30 °C, 5 MPa (TON 2.0) and 0.5 MPa, 70 °C (TON 3.0)). A final turnover number of 113 was obtained on recycling of the catalyst at 60 °C and 4 MPa of H_2/CO_2 (3:1). This catalytic system opens the door to new possibilities for hydrogenation of CO_2 to methanol under mild reaction conditions and heterogenous catalysis of molecular catalyst.

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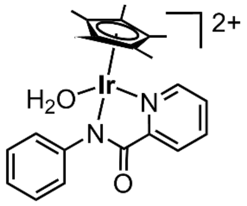
$$CO_2 + H_2 \longrightarrow CH_3OH + H_2O$$



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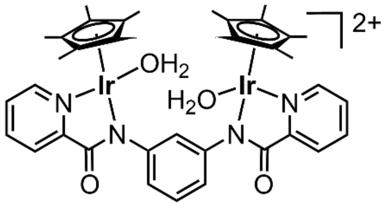

2

Table. CO_2 hydrogenation to MeOH

T / °C	P / MPa	T / h	TON
60	4	47	4.0
70	0.5	480	3.0
30	5	168	2.0
60	4	70day	113

The reaction was carried out H_2/CO_2 (3/1) using **2** in gas-solid phase reaction.

ORAL SESSION 4, LECTURE THEATRE 401-401, 30 NOVEMBER, 2023, 2.25 – 2.40 PM

CO2-blown Non-isocyanate Polyurethane Foams

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Polyurethanes (PUs) are one of the most versatile polymers having a wide range of important applications in many industries. Traditional PUs are derived from highly toxic, carcinogenic and unstable isocyanates which are in turn made using highly toxic phosgene.[1] Hence, there is a growing interest for alternative routes to PUs such as non-isocyanate polyurethanes (NIPUs) or polyhydroxyurethanes (PHUs) via polyaddition reaction between diamines and bis-cyclic carbonates, thus eliminating completely uses of phosgene and isocyanates.[2] Although NIPUs has shown promise as a replacement for traditional PU, the synthesis of NIPU foams is difficult owing to the replication of PU foaming process - in-situ CO_2 generation from isocyanate hydrolysis. In this work, we develop a method to prepare amine-CO_2 adducts and study their CO_2 adsorption and desorption under various conditions. High CO_2 desorption (up to 87%) is achieved in the adducts after aminolysis with cyclic carbonate. Next, the amine-CO_2 adduct is formulated with other monomers to obtain NIPU foams (Figure 1) with low density (0.203 – 0.239 $g.cm^{-3}$) after curing at 50 – 60 °C.

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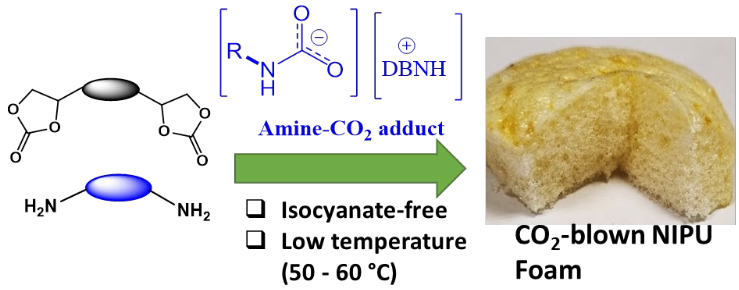

Figure 1: CO_2-blown NIPU foams.

ORAL SESSION 4, LECTURE THEATRE 401-401, 30 NOVEMBER, 2023, 2.40 – 2.55 PM

Visible-light driven fumarate synthesis using CO2 gas as a direct feedstock in a bio/photocatalytic hybrid system

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Among various plastic precursors, fumarate is a useful unsaturated dicarboxylic acid that is a plastic precursor of unsaturated polyester resin and polybutylene succinate having a good biodegradability. In contrast, current fumarate synthesis is dependent on petroleum resources, which not only emits CO_2 in the production process but also has a restriction on the resources. We have achieved the visible-light driven fumarate synthesis from HCO $^-$ and biogenic pyruvate via L-malate by applying NAD^+ photoreduction system with Zn porphyrin and Rh complex to regenerate NADH, a coenzyme of MDH, to an enzymatic reaction systemcatalyzed by two biocatalysts, malate dehydrogenase (MDH) and fumarase (FUM)[1].

However, problems with this system are that the fumarate production rate is still low and $NaHCO_3$ is used as the starting material instead of CO_2 gas causing global warming. Based on these backgrounds, we first attempted to supply HCO_3^- from CO_2 gas into the reaction system by using a weakly basic piperazine-based buffer solution. As a result, 115 mM HCO_3^- was supplied from CO_2 gas and the MDH-catalyzed reaction was successfully carried out at the maximum rate. Furthermore, we found that anionic $ZnTPPS^{4-}$, conventional photosensitizer, strongly inhibits fumarate production catalyzed by FUM. Finally, we attempted a visible-light driven fumarate synthesis from CO_2 gas and pyruvate using cationicphotosensitizer $ZnTMAP^{4+}$ with no inhibitory effect on FUM (Fig. 1). As a result, the fumarateproduction rate was successfully doubled. Thus, an efficient visible-light driven fumarate synthesis from CO_2 gas was constructed through the hybrid use of bio and photocatalysts.

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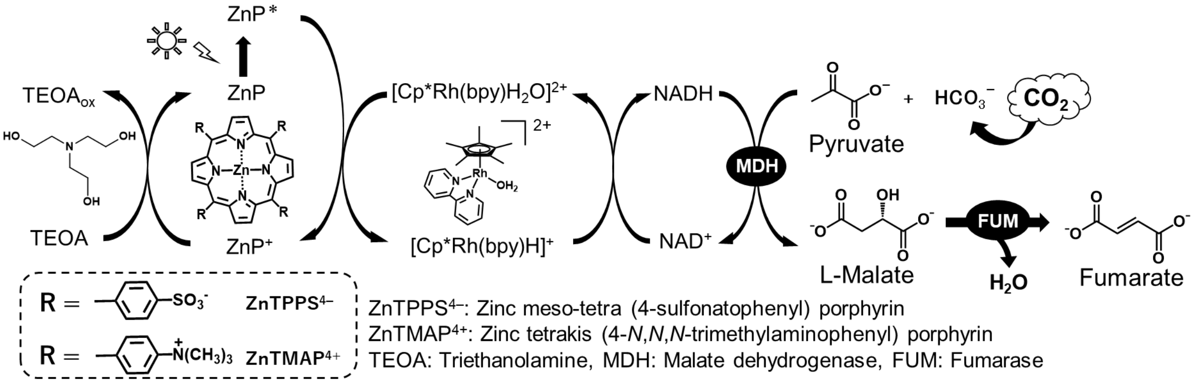

Figure 1: Visible-light driven fumarate synthesis from CO_2 gas and pyruvate by connecting NAD^+photoreduction and enzymatic reaction

ORAL SESSION 4, LECTURE THEATRE 401-401, 30 NOVEMBER, 2023, 2.55 – 3.10 PM

Hydrocarbon synthesis from CO2 using spinel oxide and zeolite

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From the viewpoint of CO_2 recycling, the tandem reactions of CO_2-to-methanol and methanol-to-hydrocarbons (MTH) have attracted attention. Although methanol synthesis from CO_2 suffers from low methanol yields due to thermodynamic equilibrium limitation, tandem reactions enable the hydrocarbons (HC) yield to exceed the equilibrium yield of methanol since methanol produced is sequentially converted to HC. In this study, mixtures of spinel oxides (AB_2O_4) and SSZ-13, an eight-membered-ring zeolite, were used as catalyst for methanol synthesis and MTH reaction, respectively. 25 different types of spinel oxides were prepared and their catalytic properties in the tandem reaction were evaluated. Catalysts obtained by physically mixing 0.5 g of spinel oxide with 0.35 g of SSZ-13 were tested for the tandem reaction in a fixed-bed reactor at 1 MPa and 653 K with the feed composition of $H_2/CO_2/N_2$=9/3/1. Fig.1 shows the product yields obtained in the tandem reaction tests. We observed that spinel oxides with Zn in A site ((Zn, B), B =Al, Cr, Fe, Ga) were found to have higher HC yields (>3.5 %). For $ZnAl_2O_4$, the calcination was performed at different temperatures,773, 873, 973 and 1073 K, and found that amorphous formed at 773 K and spinel formed above 873 K. $ZnAl_2O_4$ spinel exhibited high HC yields compared with amorphous oxide, suggesting that spinel structure is essential for the appearance of the catalytic function for methanol synthesis.

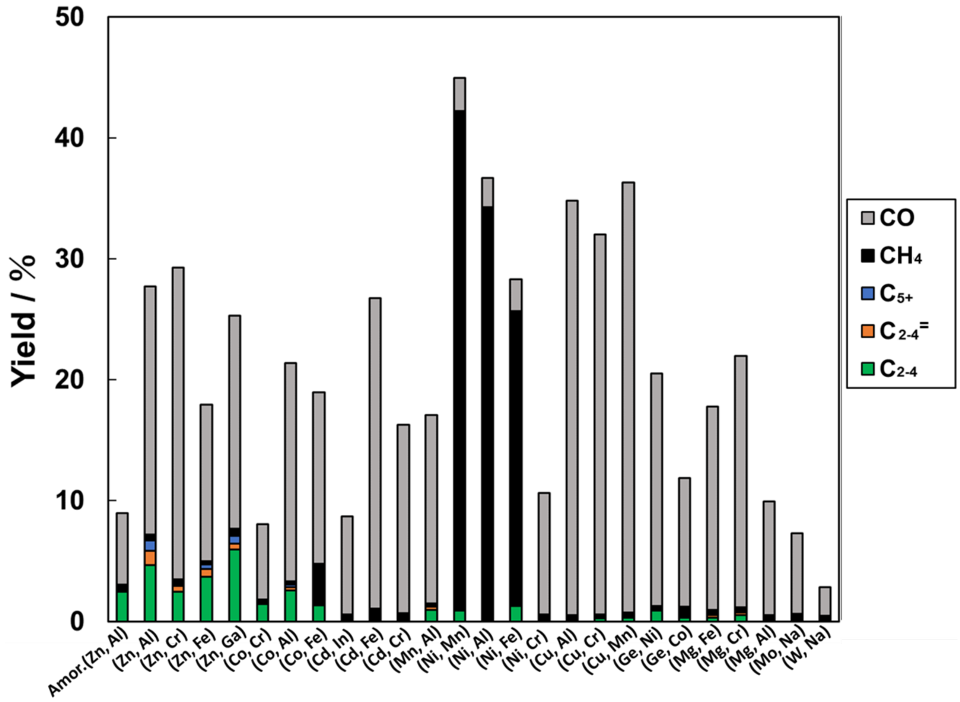

Figure 1: Product yields over various spinel oxides with SSZ-13 zeolite. Reaction conditions: $H_2/CO_2/N_2$=9/3/1, Feed rate=27 mL(STP) min^{-1}, W(AB_2O_4)=0.50 g, W(SSZ-13)=0.35 g, 1 MPa, 653 K.

ORAL SESSION 4, LECTURE THEATRE 401-401, 30 NOVEMBER, 2023, 3.10 – 3.25 PM

Applications of computational chemistry in atmospheric science

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Computational chemistry uses quantum chemistry principles and simulation approaches to understand, identify, predict, and model complex systems' structure, behaviour, and properties at a molecular level where extensive experiments may prove impractical. Furthermore, experimental results are impossible to achieve in some cases due to different limitations. This work concentrates on recent computational chemistry applications for atmospheric species on Earth, Venus, and Mars where minimal experimental results are available. The first investigated system in this work is sulfuric acid with a critical role in ozone depletion in polar regions in springtime. This molecule does not have any experimental absorption spectrum due to experimental challenges and the simulated spectrum can help scientists understand how H_2SO_4 contributes to the ozone depletion process[1]. The second investigated molecule is OSSO which was recently identified in the atmosphere of Venus. The simulated spectrum of OSSO will guide experimentalists to identify OSSO in their OSSO production investigations[2]. Additional system explored in this work is the photodissociation dynamics of the N_2O-H_2O complex and the OH radical production in the atmosphere as a byproduct. The last investigated system is the O_2 complex with ferric-oxides in the atmosphere of Mars and its possible contribution to the mysterious enhancement of the O_2 in the Martian atmosphere. These theoretical and simulated results are of significant importance whereas experimental results are almost impossible to achieve. The results of these simulations will be added to the global atmospheric database and can influence any future decision-making on these species.

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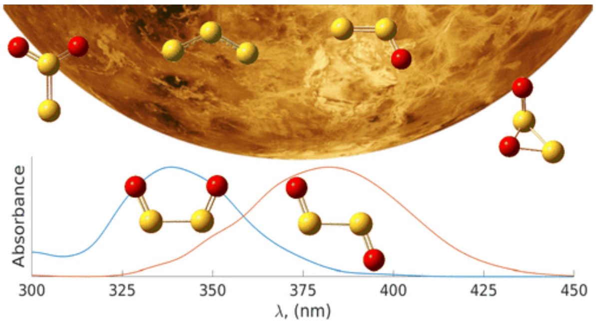

Figure 1: Simulated absorption spectra OSSO isomers[2]

ORAL SESSION 4, LECTURE THEATRE 401-439, 30 NOVEMBER, 2023, 1.30 – 1.50 PM

Atomically Dispersed Metal Catalysts Steering Selective Electrocatalysis

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Electrocatalysis is a key driver in promoting the paradigm shift from the current fossil-fuel-based hydrocarbon economy to a renewable-energy-driven hydrogen economy. The success of electrocatalysis hinges primarily on achieving high catalytic selectivity along with maximum activity and sustained longevity. Atomically dispersed metal catalysts or single-atom catalystshave emerged as a new frontier in heterogeneous catalysis. In addition to the widely perceived advantages of maximized active site utilization and substantially reduced metal content, they have shown different catalytic selectivity in some electrocatalytic reactions compared to the traditional nanoparticle-based catalysts. We have made extensive efforts toward designing carbon supported atomically dispersed metal (M–N/C) catalysts that can promote selective electrocatalysis [1]. Reactions of our interest are relevant to renewable energy conversion and commodity chemical production, including oxygen reduction reaction (ORR), hydrogen peroxide (H_2O_2) production, and chlorine evolution reaction (CER). For the ORR, tuning of metal center can direct the reaction pathway, with Fe–N/C catalyzing the ORR via the four- electron ($4e^-$) reduction to generate H_2O [2] whereas Co–N/C exhibiting preferred $2e^-$ pathway to produce H_2O_2 [3]. By combining the H_2O_2-producing Co–N/C electrocatalyst with a photocatalyst and biocatalyst (or heterogeneous catalyst), the triple catalyst systems could provide environmentally benign routes to biomass production and commodity chemical production. For the CER, Pt–N/C was found to be a highly selective catalyst that can suppress the parasitic oxygen evolution reaction (OER) [4]. The high selectivity of Pt–N/C was preserved even in low concentration of Cl^- and neutral electrolyte, under which the OER is favored. Interestingly, the Pt–N/C catalysts showed an unusual potential-dependent switching of reaction kinetics.

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ORAL SESSION 4, LECTURE THEATRE 401-439, 30 NOVEMBER, 2023, 1.50 – 2.10 PM

Chemocatalytic Synthesis of Amino Acids from Renewable Feedstocks

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Amino acids are essential compounds used in a myriad of industrial applications, including human food, animal feed, pharmaceutical products, polymer synthesis and so on.[1] Our group has developed carbon-nitrogen coupling chemistry for the synthesis of amino acids using biomass-based feedstocks as renewable carbon sources and ammonia as nitrogen source through thermal[2] and photocatalysis[3]. Here, we focus on our most recent progress – using carbon nanotubes (CNTs) as an effective catalyst for the electrocatalytic reductive amination of biomass-derivable α-keto acids into amino acids.[4] Through a facile ball milling treatment, the intrinsic defects in the CNTs were increased while the electrocatalytic activity of CNTs converting 2-ketoglutaric acid into glutamic acid was enhanced by approximately seven times. A high faradaic efficiency (FE) of ~90% with a corresponding glutamic acid formation rate of up to 180.9 mmol g^{-1}_{cat} h^{-1} was achieved, and ~60% molar yield of glutamic acid was obtained after 8 h of electrolysis. Following this protocol, a number of amino acids were prepared with moderate to high FEs and formation rates. Significantly, we synthesised long carbon chain amino acids, which are typically obtained in lower yields using the existing methods.

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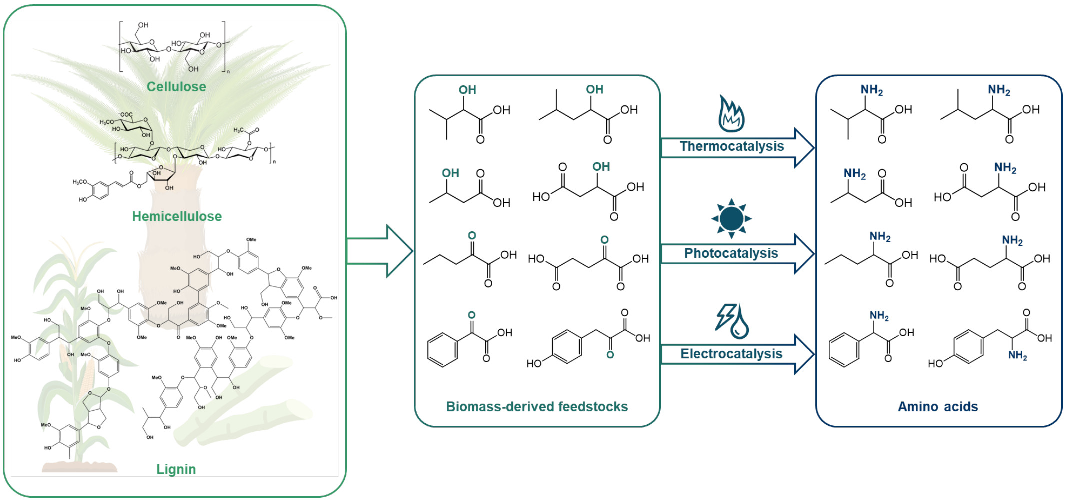

Figure 1: *Three pathways to make amino acids from renewable biomass-derived feedstocks.*

ORAL SESSION 4, LECTURE THEATRE 401-439, 30 NOVEMBER, 2023, 2.10 – 2.25 PM

Synthesis of novel photocatalysts for hydrogen and oxygen production via water splitting

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Photocatalytic overall water splitting (OWS) is a green and sustainable process that utilizes sunlight to produce hydrogen and oxygen from water. Simultaneous production of hydrogen and oxygen with a single photocatalyst is very difficult and therefore hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) photocatalysts are used in a system called Z-scheme. In this work, we synthesized Mn and Nb co-doped $BaTiO_3$ ferroelectric material for OER while cadmium sulfide (CdS) for HER. Typically, $BaTiO_3$ absorb UV light, however, after doping engineering this material can harvest visible light[1]. We investigated the OER ability with doping percentage in $BaTiO_3$ and 5% doped sample showed higher production rate. Interestingly, this is the very first report for oxygen evolution with this material. On the other hand, for HER, we prepared CdS photocatalyst with the incorporation of various amino acids. We used these compounds because the presence of an electron cloud in the organic molecules could prevent the charge recombination problem during water splitting. Among various amino acids, phenylalanine-modified CdS showed the highest production of 116 mmol/g/h. Subsequently, we varied the phenylalanine dosage from 0 to 3 mmol on CdS nanoparticles and found that 2 mmol dose exhibits superior hydrogen evolution. Moreover, we examined different amounts of photocatalyst in our laboratory-scale experimental setup, revealing that 1 mg of photocatalyst achieved an unprecedented hydrogen production rate of 221 mmol/g/h, which is 10 times higher compared to our previous report[2]. These results indicate that these two materials could be potential candidate for OWS through Z-scheme.

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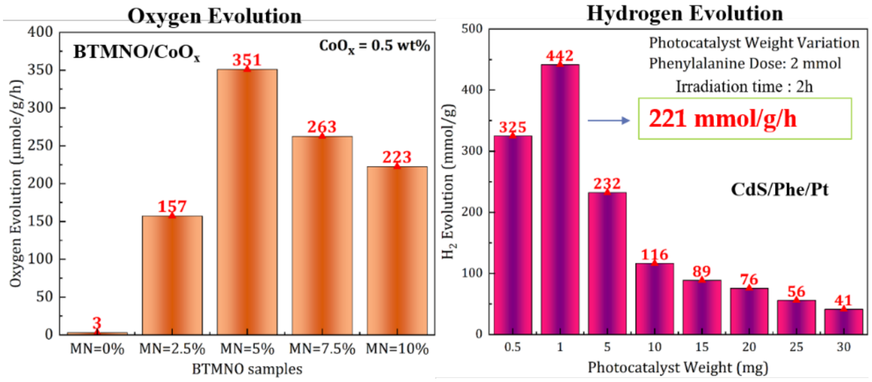

Figure: Oxygen and Hydrogen generation via photocatalytic Water splitting

ORAL SESSION 4, LECTURE THEATRE 401-439, 30 NOVEMBER, 2023, 2.25 – 2.40 PM

Eco-friendly oxygen reduction reaction electrocatalyst for high-performance green biofuel cells

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Biofuel cells have received sustained traction recently with researchers determined to provide alternative fuel sources to the otherwise expensive and pollution-prone fossil fuels. However, low output has hindered their widespread adoption. One of the proposed solutions to this bottleneck is the incorporation of an electrocatalyst on the cathode to promote the oxygen reduction reaction (ORR) hence boosting power output. Previous works have reported the use of platinum catalyst as an efficient electrocatalyst and recently our team incorporated a non-platinum group metal (N-PGM) catalyst to improve the power output in a microbial fuel cell assembly**[1]**. Despite the high performance reported, platinum materials are scarce in nature and highly costly. Similarly, transition metals that have seen their application in N-PGM face fierce competition from other day-to-day applications. This study proposes a new class of eco-friendly catalysts completely derived from waste and eco- friendly activators. The process involves hydrothermal treatment of rice husk biomass at mildconditions followed by template carbonization using NaCl as an activator and urea as a nitrogen dopant at 750 ˚C. The catalyst is then collected after neutralization using HCl. The rice husk, nitrogen-doped catalyst (RH-Fe-N-C) showed interesting properties like those of commercial catalysts (Pt/C). The catalyst in this work had an onset potential of 0.99 V, whichcorresponded to a half-wave potential of 0.856 V that was almost the same for platinum catalysts at 1.01 V and 0.839 V respectively. The eco-friendly synthesized catalyst presents a cheaper and environmentally friendly catalyst that can substitute the otherwise expensive metal-derived electrocatalysts.

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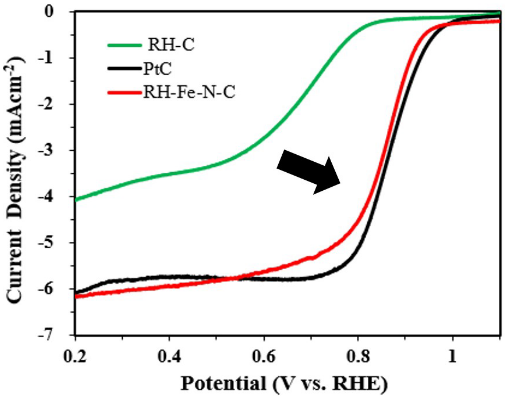

Catalyst	E_{ONSET} (V)	Limiting current density $|J_{lim}|$ mA/cm^2	Transfer electrons	Reference
RH-Fe-N-C	**0.99**	**5.81**	**3.9**	**This work**
Si-Fe/S/N-RH$_3$	*0.96*	*5.23*	*3.9*	*F. Wang et al 2022*
FeTPP/RHC	*0.96*	*4.50*	*3.7*	*Xie W-Y et al 2023*
N-RHPC	*0.93*	*5.50*	*3.9*	*Jun Shi et al 2020*
RHFeN	*0.87*	*~2.00*	*-*	*H. Jin et al 2023*
RH-C	**0.85**	**3.30**	**3.0**	**This work**
DKCoN-900	*0.69*	*2.00*	*3.5*	*H. Jin et al 2021*
PtC	**1.01**	**5.79**	**4.0**	**This work**

Figure: ORR activity performance as compared to other reported rice husk-derived catalyst

ORAL SESSION 4, LECTURE THEATRE 401-439, 30 NOVEMBER, 2023, 2.40 – 2.55 PM

Mechanistic study on electro-oxidation of 5- hydroxymethylfurfural and water molecules via operando surface-enhanced Raman spectroscopy coupled with an Fe3+ probe

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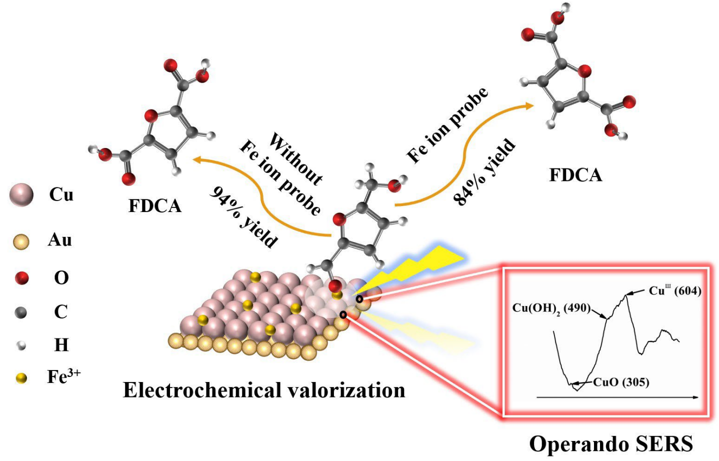

Figure: Effects of adding iron ions on the HMF electro-oxidation reaction.

Electrocatalytic oxidation of biomass such as 5-hydroxymethylfurfural (HMF) is a green route to produce value added chemicals. However, in-depth understanding of the electrocatalytic process is still lacking. Herein, the mechanism of HMF electro-oxidation was studied by operando surface-enhanced Raman spectroscopy (SERS) coupled with an Fe^{3+} probe. A multicomponent platform consisting of titanium plates integrated with a gold film and uniform nickel and copper nanoparticles (NPs) was employed as an electrode as well as a SERS substrate, enabling operando SERS study on the electrocatalytic process with simultaneous evaluation on catalytic activity and visualization on the variations of active sites. Fe^{3+} was intentionally added into the electrolyte as a probe to correlate the nature of active sites with catalytic activity and product selectivity in virtue of its strong interaction with the active sites of the electrocatalysts. Electrodes integrated with Ni and Cu NPs exhibited excellent HMF oxidation performance but their activity were suppressed by adding 1 ppm Fe^{3+}. Conversely, the activity towards water oxidation was significantly enhanced by Fe^{3+} addition. Fe^{3+} inhibitsthe oxidation of Ni^{2+} to Ni^{3+} and promotes the formation of more CuO and Cu^{3+}. Cu^{3+} is a better active site for water oxidation. A highest 2,5-furandicarboxylic acid yield (94.0%) and a maximum HMF conversion (98%) were obtained from the electrode integrated with Cu NPs at a potential of 1.47 V. This work affords a feasible route to explore mechanisms of electrocatalytic processes.

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ORAL SESSION 4, LECTURE THEATRE 401-439, 30 NOVEMBER, 2023, 2.55 – 3.10 PM

Polyethylene decomposition over zeolite catalysts in hydrocarbon solvents

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Chemical recycling technology is necessary for converting waste plastics into chemical raw materials. We propose a cracking process using zeolites as catalysts, dissolved in a hydrocarbon solvent to reduce the viscosity of the fluid containing the plastic, to promote heat transfer in the process, and to allow the removal of foreign substances such as additives.

Using a 100 cc batch reactor, 5.0 g of LDPE, 20 g of solvent (n-C16, 1-M.N.), and 0.25 or 1.0 g of Beta zeolite were reacted at 400°C for 1 h. Fig. 1 shows the comparison of results using n-C16 and 1-M.N. solvents and the product yields with and without PE, respectively. In this study, the denominator of yield was calculated as solvent (20 g) + catalyst (1 g), so that the maximum total yield was 124% for the case with PE (5 g). When n-C16 was used as a solvent, PE was decomposed satisfactorily. C3~C9 components were obtained from PE. However, when 1-M.N. was used, PE conversion was lower.

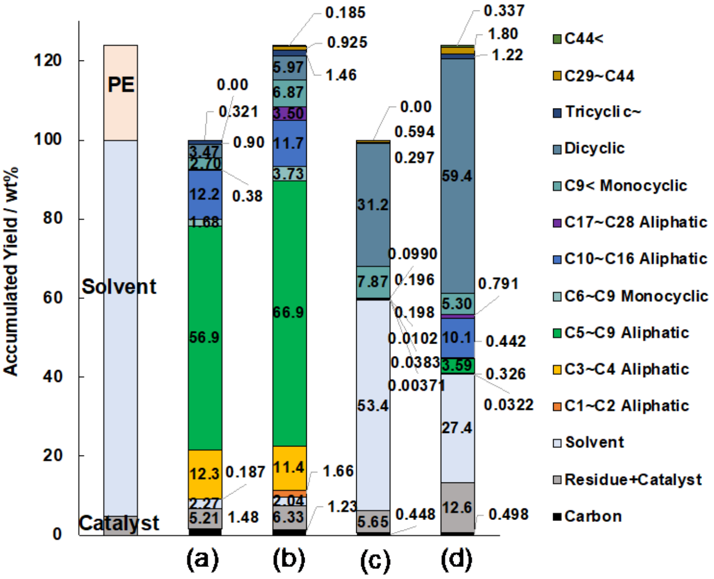

Figure 1: PE decomposition results in *n*-C16 and 1-M.N. over beta (400 °C, 60 min, Beta: 1.0 g). (a) n-C16 +Beta, (b) n-C16 + PE + Beta, (c) 1-M.N. + Beta, and

As shown in Table 1, HDPE showed a higher conversion. This is likely because HDPE has aless branched structure than LDPE and can penetrate into the pores of Beta more easily. PEitself may penetrate into the pores of Beta and undergo decomposition.

In conclusion, PE can be decomposed to C3-C9 hydrocarbons, especially in aliphatic solvents. Zeolite is interesting in its catalytic behavior for PE decomposition.

Table 1 Decomposition results of HDPE and LDPE

	Decomposition Temperature/°C	PE conversion/%	n-C16 conversion/%
LDPE	452	78.9	76.4
HDPE	465	94.3	72.9

KEYNOTE SESSION 3, LECTURE THEATRE 401-401, 30 NOVEMBER, 2023, 4.00 – 4.30 PM

Green chemistry enabled synthesis of aminated responsive materials

Laurel L. Schafer[1]

[1] *Department of Chemistry, The University of British Columbia*

[2] *Organisation*

The development of a general catalyst for the catalytic synthesis of selectively substituted amines from amines and alkenes has been realized. Hydroaminoalkylation is an alkene hydrofunctionalization reaction that adds an activated C_{sp}^3-H bond α-to N across an alkene to generate a new C_{sp}^3 – C_{sp}^3 bond.[1] This solvent-free reaction can be completed on multigram scale and avoids the installation of amine protecting/directing groups. These patented catalysts, with TONs up to >200 h, can be used in materials chemistry applicationsto access a new class of aminated materials.[2,3] The resultant materials show remarkable self-healing and adhesion properties to diverse surfaces including PTFE (Teflon™). They also show promising anti-corrosion properties that work underwater, including in marine environments. This talk will describe how fundamental developments in bond activation and catalysis can be leveraged to realize materials science inventions – aminated polyolefins - that show promise as new underwater adhesive technologies and anti-corrosion coatings.

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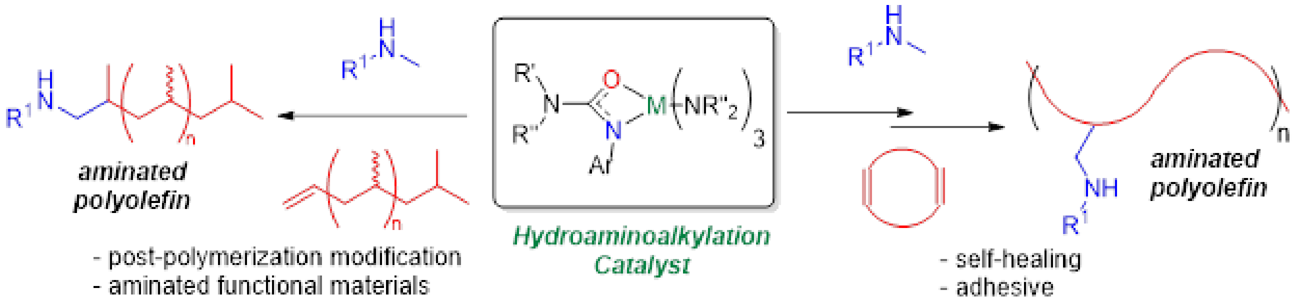

Figure: Hydroaminoalkylation catalysts enable the synthesis of two distinct classes of aminatedpolyolefins.

KEYNOTE SESSION 4, LECTURE THEATRE 401-401, 30 NOVEMBER, 2023, 4.30 – 5.00 PM

BTEX from Lignin using a Novel Molybdenum Carbo-nitride@Titanium Nitride Catalyst

Matthew Y. Lui[1], Alexander K.L. Yuen[2], Stuart Bartlett[3], Anthony F. Masters[2], Thomas Maschmeyer[2]

[1] *Department of Chemistry, Hong Kong Baptist University, Hong Kong*

[2] *School of Chemistry, The University of Sydney, Sydney, 2006, Australia*

[3] *Diamond Light Source, Harwell Science & Innovation Campus, Didcot, Oxfordshire OX110DE, UK*

After a short general overview of the Cat-HTR process for the upgrading of waste biomass and its key transformations, interrogated by model compounds studies, this talk will focus on what might be an evolution of this process that is currently being commercialised with a 20,000 tpa plant being built in Canada.

This evolution includes the addition of *in-situ* reduction agents and will discuss the key structural features and compositional aspects of several molybdenum hemicarbide-based catalysts using a combination of synchrotron techniques, X-ray diffraction and elemental mapping in conjunction with electron microscopy [1] as well as their catalytic performance in the conversion of lignin to BTX using supercritical ethanol and base. [2]

The molybdenum hemicarbides as well as a molybdenum carbo-nitride composite material were prepared by thermal decomposition of a molybdenum–melamine polymer in the presence of titanium nitride at 650 °C under a reducing atmosphere. The catalytic reactions were performed in supercritical ethanol at between 280 and 330 °C and the samples anaylsed using a variety of spectrocopic and chromatographic techniques.

The composite was shown to be more effective than either Mo_2C or Mo_2N for the hydrodeoxygenation of lignin to single-ring arenes in supercritical ethanol. Extended X-rayabsorption fine structure experiments at 330 °C, under a stream of ethanol vapor to approximate in situ conditions, elucidate the importance of the interaction of the titanium nitride support with the molybdenum carbo-nitride phase. The titanium nitride and molybdenum carbide phases are intimately intergrown.

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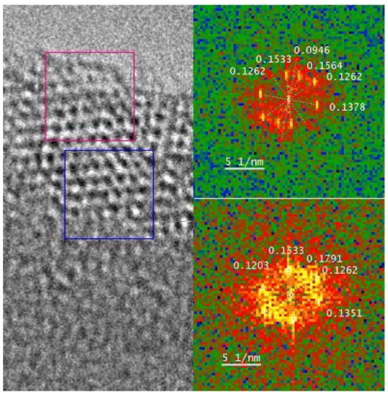


Figure: Double aberration corrected TEM of $Mo_2C_xN_{1-x}$@TiN

ORAL SESSION 5, LECTURE THEATRE 401-401, 1 DECEMBER, 2023, 9.30 – 9.50 AM

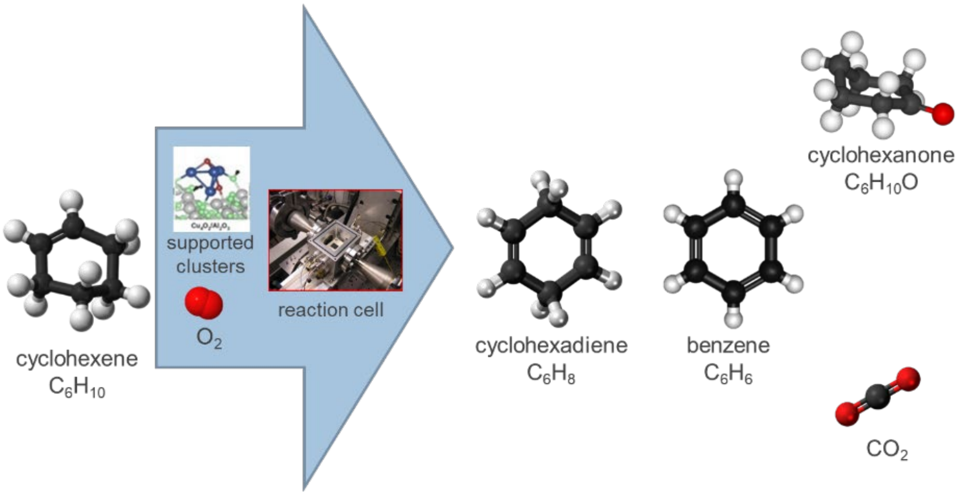
Shifting Catalytic Activity and Selectivity Atom-by-Atom by Subnanometer Cluster Catalysts

Stefan Vajda

Department of Nanocatalysis, J. Heyrovsky Institute of Physical Chemistry,

Czech Academy of Sciences, Dolejskova 2155/3, 182 23 Prague, Czech Republic

The focus of the presentation will be on catalysis by supported monodisperse subnanometer clusters made of a handful of atoms, supported on technologically relevant oxide- and model carbon-based supports. The performance of Co, Cu, Pd and CuPd clusters on the example of oxidative dehydrogenation of cyclohexene where an atomic precision fabrication of mono- and bimetallic clusters allows for the fine-tuning of their activity and selectivity by varying the size and composition of the clusters in an atom-by-atom fashion and by support effects.



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ORAL SESSION 5, LECTURE THEATRE 401-401, 1 DECEMBER, 2023, 9.50 – 10.10 AM

Addressing hydrocarbon separations using MOFs as a bottom- up approach towards energy alternatives

Lauren K. Macreadie,[1]

[1]*University of New South Wales, Kensington, NSW, Australia*

The growing global interest into finding alternative energy sources has seen impressive developments over recent years. Our research team is focussed on a bottom-up approach for decreasing our reliance on fossil fuels and decreasing CO_2 emissions. The bottom-up approach focusses on individual technologies which ultimately rely upon fuels for function. For example, the purification of hydrocarbons is a highly important process, however the distillation methods often employed to separate these are energy intensive and expensive and account for 10 – 15 % of the worlds energy consumption. Therefore, applying methods which could mitigate these processes could save 100 million tonnes of carbon dioxide emissions each year.[1]

Highly porous metal-organic frameworks (MOFs) are the leading class of adsorbent materials and have huge potential to address these challenges. MOFs and other porous materials are excellent alternatives to this high energy process as these do not require fuel driven distillation purposes to separate industrially important hydrocarbon mixtures. Here, presents our research on the use of commercially available 3D-linkers to form 3D-Linker MOFs (3DL-MOFs) and investigate their hydrocarbon separation properties. Through the incorporation of 3D-linkers into prominent MOF architectures, we demonstrate the striking effects a contoured, aliphatic pore environment has on gas and hydrocarbon adsorption, compared with its aromatic counterpart, and explore the potential separation capacities these frameworks may pose.[2,3] 3DL-MOFs show enhanced selectivity and separation behaviour over their aromatic counterparts due to the highly contoured surface of the pore and the extra functionalities which protrude from the linker body into the MOF cavity.

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ORAL SESSION 5, LECTURE THEATRE 401-401, 1 DECEMBER, 2023, 10.10 – 10.25 AM

Photocatalytic Hydrogen Peroxide Production Utilizing Al- Based Metal-Organic Frameworks

Yoshifumi Kondo,[1,2] Kenta Hino,[1] Yasutaka Kuwahara,[1] Kohsuke Mori,[1] Hiromi Yamashita[1]*

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Hydrogen peroxide (H_2O_2) has attracted much attention as a promising liquid fuel as well as an eco-friendly oxidant. Photocatalytic process is a sustainable method to generate H_2O_2 from earth abundant O_2 in response to sunlight. In the photocatalytic H_2O_2 production, the undesired H_2O_2 decomposition over photocatalysts is a substantial drawback [1-3]. Aluminium oxides are almost inert to H_2O_2 decomposition, but their wide band gap energy makes them unsuitable as a photocatalyst. Interestingly, benzyl alcohol oxidation with Al_2O_3 and photosensitizers has been suggested to produce H_2O_2 as a reduction product. Therefore, we anticipated that the hierarchical integration of photosensitizing amine- functionalized organic linkers with Al-oxo clusters into the matrix of metal-organic frameworks (MOFs) would lead to a photocatalyst with exceptional performance in H_2O_2 production by suppressing H_2O_2 decomposition [4]. Figure 1 shows H_2O_2 production over Al- MOFs (Al-MIL-101-NH_2, Al-MIL-53-NH_2, and Al-CAU-1) under visible-light irradiation. Al-MIL- 101-NH_2 exhibited the highest activity toward H_2O_2 production among Al-MOFs, indicating that the framework of MIL-101-NH_2 is critical to achieve effective photocatalytic H_2O_2 production. Furthermore, when the H_2O_2 decomposition test was conducted in the dark, the initial concentration of H_2O_2 was maintained in Al-MIL-101-NH_2. Thus, Al-MIL-101-NH_2 functions as a photocatalyst that continuously produces H_2O_2 with little H_2O_2 decomposition.

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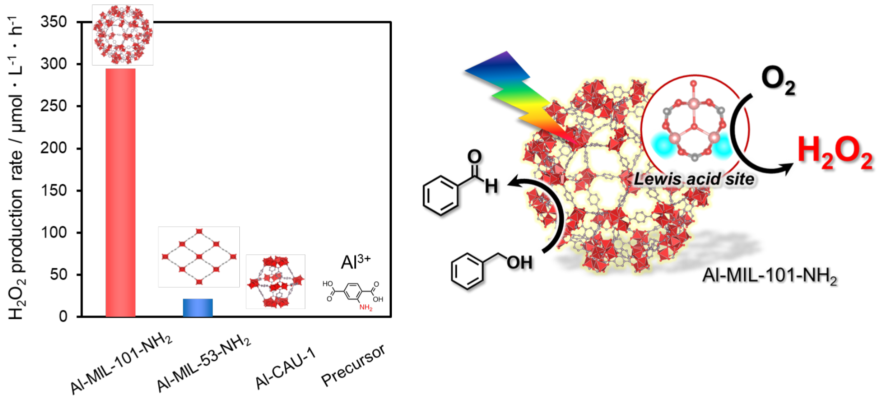

Figure 1: Comparison of photocatalytic H_2O_2 production over Al-MOFs in an O_2-saturated acetonitrile solution containing benzyl alcohol under visible-light (λ > 420 nm) irradiation.

ORAL SESSION 5, LECTURE THEATRE 401-439, 1 DECEMBER, 2023, 9.30 – 9.50 AM

Catalytic Asymmetric Synthesis of Chiral Indole Derivatives

Feng Shi[1,2]

[1]*School of Chemistry and Materials Science, Jiangsu Normal University, Xuzhou 221116,China, fshi@jsnu.edu.cn*

[2]*School of Petrochemical Engineering, Changzhou University, China, Changzhou, 213164,China, fshi@cczu.edu.cn*

Chiral indole derivatives are wide found in many natural products, pharmaceuticals, and chiral catalysts or ligands. So, the catalytic asymmetric synthesis of chiral indole derivatives has absorbed great attention from the scientific community. However, there are still some challenges in the synthesis of chiral indole derivatives. For example, limited asymmetric organocatalysis, limited types of platform molecules, and limited catalytic asymmetric reactions have been developed for the synthesis of chiral indole derivatives. Therefore, new strategies to solve these challenging issues are highly needed. To confront these challenges, our group developed a unique strategy of designing and developing platform molecules and their involved organocatalytic asymmetric reactions (Figure 1).[1] Based on this strategy, we have synthesized a wide range of indole-based chiral heterocycles bearing either central chirality and/or axial chirality.[2] In this talk, the recent progress of our group in chiral indole chemistry will be presented.

References

1. For summaries on our work in chiral indole chemistry: a) Zhang, Y.-C.; Jiang, F.; Shi, F. *Acc. Chem. Res.* 2020, *53*, 425; b) Zhang, H.-H.; Shi, F. *Acc. Chem. Res.* 2022, *55*, 2562.
2. For recent examples: a) Ma, C.; Sheng, F.-T.; Wang, H.-Q.; Deng, S.; Zhang, Y.-C.; Jiao, Y.; Tan, W.; Shi, F. *J. Am. Chem. Soc.* **2020**, *142*, 15686; b) Sheng, F.-T.; Yang, S.; Wu, S.-F.; Zhang, Y.-C.; Shi, F. *Chin. J. Chem.* **2022**, *40*, 2151; c) Chen, K.-W.; Chen, Z.-H.; Yang, S.; Wu, S.-F.; Zhang**,** Y.-C.; Shi, F. *Angew. Chem., Int. Ed.* **2022**, *61*, e202116829; d) Chen, Z.-H.; Li, T.-Z.; Wang, N.-Y.; Ma, X.-F.; Ni, S.-F.; Zhang, Y.- C.; Shi, F. *Angew. Chem., Int. Ed.* **2023**, *62*, e202300419; e) Zhang, J.-Y.; Chen , J.- Y.; Gao, C.-H.; Yu, L.; Ni**,** S.-F.; Tan, W.; Shi**,** F. *Angew. Chem., Int. Ed.* **2023**, *62*, e202305450.

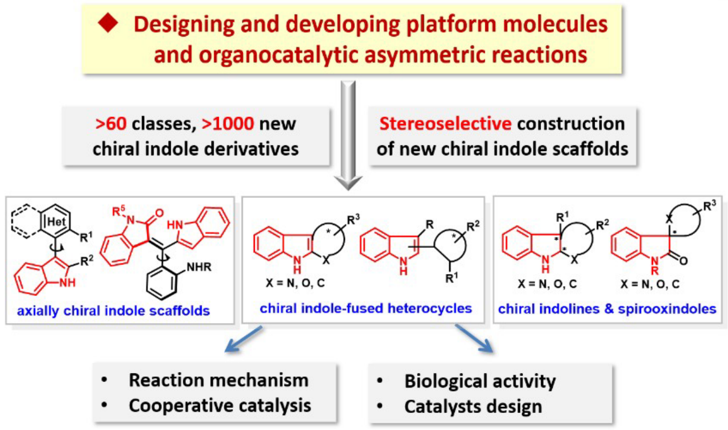

Figure 1. Our strategy for catalytic asymmetric synthesis of chiral indole derivatives

ORAL SESSION 5, LECTURE THEATRE 401-439, 1 DECEMBER, 2023, 9.50 – 10.10 AM

Flow-enabled photosensitized [2+2] cycloadditions for the synthesis of natural products.

Zoe E. Wilson, Saawan Kumar, David Barker and Christopher Larsen

School of Chemical Sciences, University of Auckland

[2+2] Cycloadditions powered by visible light sensitised triplet energy transfer have immense, but largely unexplored potential for the concise and green synthesis of complex natural products, which have been hitherto limited by the requirement of harsh UV irradiation.[1] The rapid expansion of visible light sensitised photochemistry necessitates similar progress in photoreactor design. Flow-enabled photochemistry offers many advantages over traditional batch photoreactors, including efficient and uniform irradiation throughout the reaction mixture, precise temperature control, scalability and facile in-line monitoring.[2]

N-methylflindersine (**1**) and bergapten (**2**) are the proposed biosynthetic precursorsof the bioactive natural products melicodenine F (**3**), G (**4**) & J (**5**), with the symmetrical bergapten dimer **6** also having been isolated from nature.[3] The large range of feasible combinations of these molecules represents an intriguing challenge (Figure). We have developed an in-house flow photoreactor and herein report initial investigations into the reactivity, selectivity and tunability of the flow-enabled visible light sensitised [2+2] cycloaddition of **1** and **2.**

References

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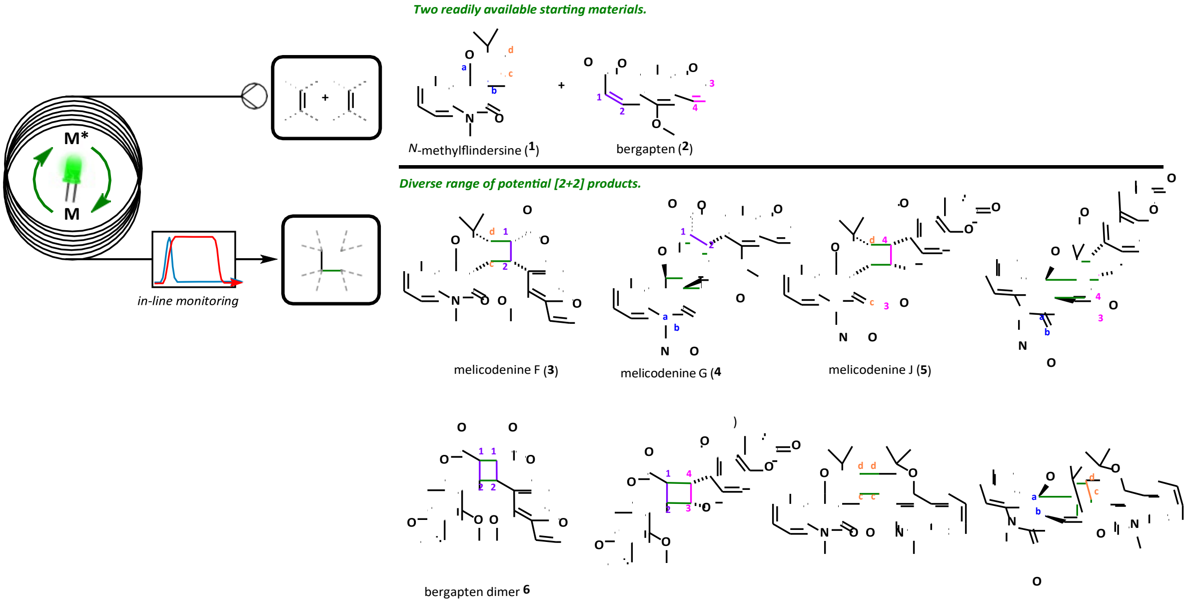

Figure: Using flow photochemistry to probe the synthesise of cyclobutane containing products from *N*-methylflindersine (**1**) and bergapten (**2**).

ORAL SESSION 5, LECTURE THEATRE 401-439, 1 DECEMBER, 2023, 10.10 – 10.25 AM

Highly Active and Chemoselective Homobimetallic Ruthenium Catalyst for One-pot Reductive Amination in Water

Gopal Deshmukh, Thakur Rochak Kumar Rana, Nikita Yadav, Gopalan Rajaraman and Ramaswamy Murugavel*

Department of Chemistry, Indian Institute of Technology Bombay, Mumbai 400 076, India.

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Amines are essential in organic synthesis as well as in various industries, prompting significant efforts to develop efficient catalytic system. Reductive amination (RA) reactions between carbonyl compounds and amines catalysed by transition metal complexes offer an efficient route to amine synthesis.[1] Keeping in mind, two new Ru(II) compounds, homobimetallic (**Ru1**)and monometallic (**Ru2**) incorporating Schiff base ligands have been synthesised.[1, 2] Both complexes are water/air-stable at room as well as high temperatures, were employed as catalysts for RA in water using formate buffer as the hydrogen source. Complex **Ru1** catalyses one-pot RA for the production of secondary amines in ~99% yield with TON and TOF of 4.3×10^4 and 107×10^3 h^{-1}, respectively and is the highest reported for any RA reactions. A comparative study between **Ru1** and **Ru2** reveals that complex **Ru1** exhibits better chemoselectivity for the formation of the secondary amines, attributable to a cooperative effect. This cooperative effect has been further substantiated through extensive DFT calculations on bimetallic and monometallic Ru(II) complexes along a hybrid-model complex.

References

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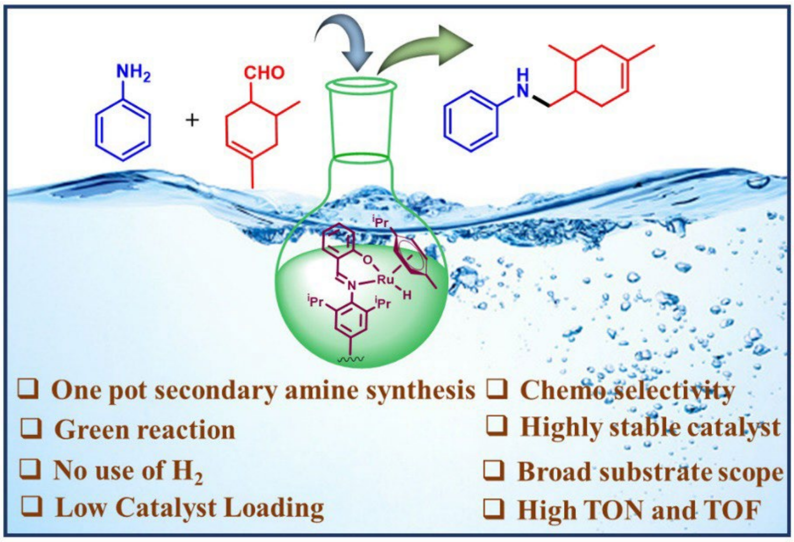

KEYNOTE SESSION 5, LECTURE THEATRE 401-401, 1 DECEMBER, 2023, 11.00 – 11.30 AM

Green Chemistry Education: A Fundamental Theoretical Perspective with Augmented Reality Integration for Enhanced Delivery

Mageswary Karpudewan

School of Educational Studies,

Universiti Sains Malaysia, Penang.

Green chemistry, once primarily applied in industrial settings, is now finding its way into educational contexts. The incorporation of green chemistry principles into teaching and learning across all levels has been realized through the utilization of the twelve guiding principles in laboratory experiments. These principles have also been seamlessly integrated into the teaching of scientific concepts. While the integration of green chemistry has yielded positive results and serves as an exemplary model for educators, teaching green chemistry is often perceived as challenging due to the significant curriculum changes it entails. To address this challenge, a comprehensive mixed-method study was undertaken to propose the implementation of green chemistry based on a robust theoretical foundation. Activity Theory, initially rooted in classical German philosophy and now a thriving multidisciplinary field, serves as the mediating force for behavioural change. The theory delineates activity into six components subject, object, tools, rules, community, division of labour, and outcomes. By presenting green chemistry principles within the framework of Activity Theory,subjects are guided to distribute tasks according to established rules, resulting in the generation and dissemination of knowledge throughout the community. This Activity Theory-based approach to teaching green chemistry was rigorously tested with 186 pre-university students. This proposed strategy effectively addresses the prior lack of a strong theoretical foundation in the implementation of green chemistry within the realm of education and stands as a valuable guide for educators. Furthermore, this approach opens up new possibilities for the integration of Augmented Reality (AR) in teaching, presenting intriguing implications for education.

ORAL SESSION 6, LECTURE THEATRE 401-401, 1 DECEMBER, 2023, 11.30 – 11.50 AM

Green chemistry in higher education: An upstream approach to addressing sustainable development goals.

Amy S. Cannon

Beyond Benign, Wilmington, MA, USA

The field of chemistry has a critical and foundational role in addressing the SustainableDevelopment Goals outlined by the United Nations [1]. Green chemistry provides chemists with principles and a framework to design chemical products and processes that reduce or eliminate hazards and impacts [2]. Chemists have made significant positive impacts on society through the design of sustainable chemistry technologies [3]. Unfortunately, our current global education systems do not properly prepare most scientists to select and design sustainable chemicals, processes, materials, and products. Green chemistry education addresses sustainability at the earliest stages of the value chain, maximizing impacts. Undergraduate and graduate level training is an essential stage in the training of scientists and professionals that are prepared with the skills to address hazards and mitigate impacts at the design stage of a product lifecycle[4].

This presentation will provide an overview of the opportunities that green chemistry provides for college and university faculty to prepare students with 21st century skills to address sustainability through chemistry. Beyond Benign, a non-profit organization dedicated to green chemistry education, programs will be highlighted, including the Green Chemistry Commitment, a consortium program for university chemistry departments to adopt green chemistry in their teaching practices. Academic models foradopting green chemistry in education and research will be included. The new Green Chemistry Teaching and Learning Community (GCTLC) will also be discussed, an open-source, on-line platform for the global green chemistry community to share resources, collaborate and network to improve their teaching and practice of green chemistry.

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ORAL SESSION 6, LECTURE THEATRE 401-401, 1 DECEMBER, 2023, 11.50 AM – 12.10 PM

Temperature control strategy in a flow reactor for safer operation and higher heat efficiency

Yosuke Muranaka[1], Taisuke Maki[1], Kazuhiro Mae[1]

[1]Department of Chemical Engineering, Kyoto University

In recent years, flow synthesis has been gradually replacing batch production system, especially in the field of high value-added chemical production such as pharmaceuticals and cosmetics. In particular, the use of microreactors is expected to enable rapid mixing, precise temperature control, and rapid start-up, resulting in more energy-efficient synthesis. For example, Kawaguchi *et al.* introduced a process with higher yield and selectivity at room temperature by precisely controlling the temperature in a microreactor, which required low temperature conditions such as -70°C in a batch reactor [1]. In this presentation, previous studies which precise temperature control contributed to improving the reaction performancewill be introduced. Next, guidelines for temperature control in the reactor for safer and more thermally efficient operation will be presented. The new dimensionless number β was proposed, which expressed the ratio of heat generation rate to heat transfer rate. The relationship of β and $\Delta T_{\mathrm{max}}/\Delta T_{\mathrm{ad}}$, which is standardized maximum temperature change in thereactor by adiabatic temperature change, was confirmed to follow the same proportional line,with several different physical values of the system. According to the equation, the allowablereactor properties such as a diameter could be determined under the desirable temperature change, and the usefulness was validated.

Reference

1. T. Kawaguchi, H. Miyata, K. Ataka, K. Mae, J. Yoshida, *Angew. Chem. Int. Ed.* **2005**, *44*, 2413-2416.

Acknowledgement: This presentation is based on results obtained from a project subsidized by the New Energyand Industrial Technology Development Organization (NEDO).

ORAL SESSION 6, LECTURE THEATRE 401-401, 1 DECEMBER, 2023, 12.10 – 12.30 PM

Applied research in green and sustainable chemistry: a Singapore story

Valerio Isoni

Singapore Institute of Technology

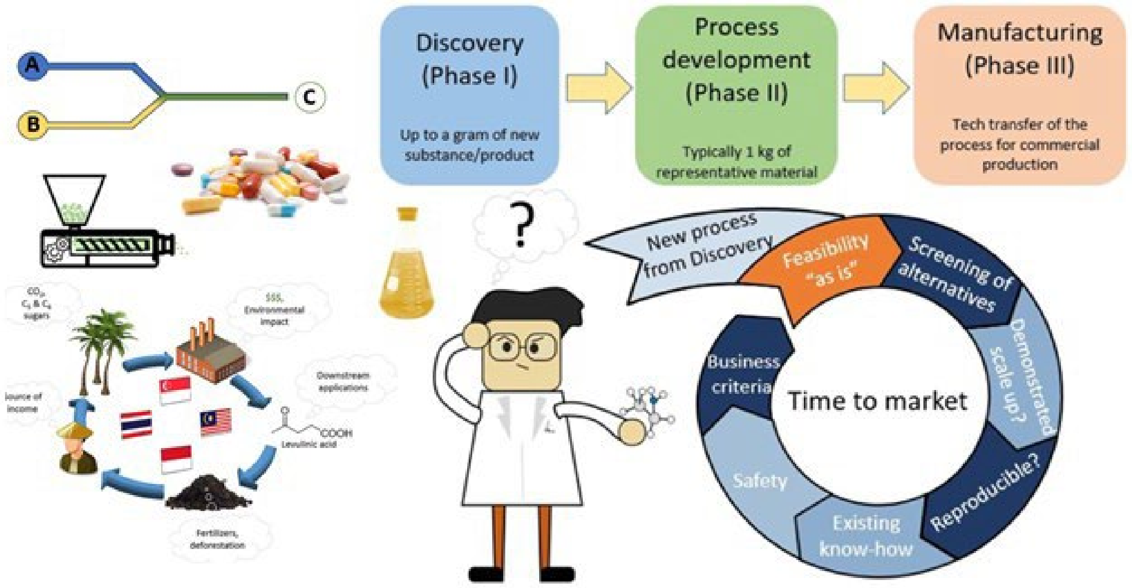

Figure: Applied research in green chemistry and engineering

This presentation features untold stories from Singapore in green and sustainable chemistry. The talk showcases applied research examples over the span of a decade, ranging from green metrics and life cycle assessment tools developed for Pharma, techno-economic evaluation of biomass-to-chemicals in Southeast Asia, novel catalytic systems tested under simulated process conditions, and green engineering approaches that have effectively solved industrial challenges locally and/or internationally. Tackling organic solvent use by elimination and/or substitution we reduced waste, and improved safety and productivity in commercial processes. By embracing technologies such as continuous flow reactors, we have witnessed remarkable enhancements in productivity, coupled with reduced resource consumption and energy efficiency. We challenged the *status quo* for multiphasic reactionsat scale using unconventional reactors for exothermic transformations. The successful integration of these approaches has been instrumental in resolving industrial challenges, paving the way for cleaner and more sustainable chemical production. Water-based chemistry, process intensification, continuous chemical processing and cleaning strategies are among some of the continuously growing areas of applied research hinging on green chemistry and engineering principles that I will share with you, illustrating how these principles can be harnessed to address the complex challenges facing the chemical industry.

There are various options for green and sustainable chemistry enthusiasts beyond the well-trodden path – come and hear from a former synthetic chemist gone multidisciplinary to know more!

ORAL SESSION 6, LECTURE THEATRE 401-439, 1 DECEMBER, 2023, 11.30 – 11.50 AM

Study of Decarbonisation on the Special Remote Area in East Indonesia

Eniya Listiani Dewi[1], Khotimatul Fauziah[1], Toha Zaky[1], Kurniawan[2], Hamid Budiman[1]

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[2]Indonesia Fuel Cell and Hydrogen Energy (IFHE), Indonesia

The implementation of sustainable and low-carbon technologies and practises is essential for decarbonization. This necessitates a considerable transition away from conventional manufacturing and energy-use techniques, which have depended mainly on fossil fuels. Several steps can be taken in a variety of industries, for instance in Indonesia, to accomplish decarbonization. First, there needs to be a major expansion in the capacity of geothermal, solar, and wind energy to enable greater use of renewable energy sources. Second, phasing out the majority of coal-based energy generation, which accounts for more than 75% of greenhouse gas emissions, is a key step. The actual application of the co-firing method Maintaining the current natural gas generating capacity is crucial to ensuring dependability.

Another crucial element is shifting to a more environmentally friendly transport sector with the intention of raising the proportion of zero-emission automobiles. Strict energy efficiency regulations for new structures and appliances will also aid in lowering energy consumption. To reduce emissions from industrial processes and transportation, research and development activities should concentrate on CCS and CCUS technologies, as well as carbon-neutral fuels (biodiesel, bioethanol, etc.), and green hydrogen. To assist the shift to a low- carbon economy, infrastructure development for power and pipelines made especially for CO2 and hydrogen gas is also required. Significant progress can be achieved in decarbonizing islands by putting these strategies into place.

Small-scale microgrids using hydrogen and fuel cell technology, instead of diesel, require a greater photovoltaic (PV) capacity since they are less efficient, according to the implementation scenario of de- dieselization that was studied in the small island of Semau-East in Indonesia. Electrolyzers, hydrogen tanks, and fuel cells need to be integrated on a wider scale if CO2 emissions are to be significantly reduced (up to 60%) and diesel use is to be reduced. However, compared to the current system, this strategy nearly doubles the cost of generation. Furthermore, there is some complexity in the link between fuel cell efficiency and CO2 reduction, as fuel cells operating at 60% efficiency may reduce CO2 at a lower rate than those operating at 40% or 80% efficiency. The study emphasises that as renewable microgrids entirely rely on PV output, fluctuations in CO2 emissions are primarily determined by the magnitude of the PV capacity.

ORAL SESSION 6, LECTURE THEATRE 401-439, 1 DECEMBER, 2023, 11.50 AM – 12.10 PM

Molecular electron acceptors and the new photophysical landscape of organic solar cells

Paul Hume,[1,2] Sai Shruthi Murali,[1,2] Michael B. Price,[3] Justin M. Hodgkiss[1,2]

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Organic solar cells / photovoltaics (OPVs) are a promising technology for the utilisation of the most abundant renewable energy source: sunlight. Efficient light absorption enables organic photovoltaics to be ~1000 times thinner than traditional silicon solar cells, making them lightweight, flexible, and versatile. However, organic solar cells don't convert sunlight into electricity as efficiently as silicon technologies. Improvements in OPV efficiency are primarily driven by the discovery of new materials with improved photophysics. This is particularly true of the past decade, which has seen the rise of a new generation of materials known as 'fused-ring' electron acceptors (FREAs). These materials have propelled OPV efficiency to >19 % due to their exceptional intrinsic properties that have altered the processes responsible for light-to-electricity conversion. This talk will briefly survey our recent contributions to understanding the novel photo-physics of FREAs, including:

- The discovery of direct electric charge formation in a single component FREA material, unlike previous generations of OPV materials which require two distinct organic materials.[1]
- The identification ability of 'slow' processes that could previously be neglected, suchas intersystem crossing, that are now able to compete with charge formation.[2]
- Our efforts to understand and model the rapid, long range energy transfer that occursin FREAs, with the aim of enabling high-throughput virtual screening of organic semiconductor materials.[3]

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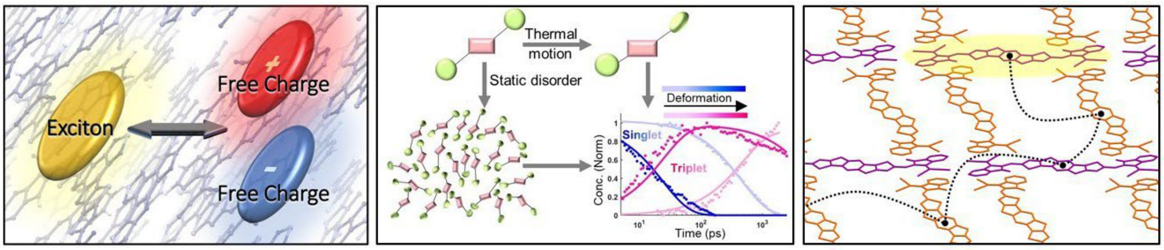

Figure: (a) Intrinsic electric charge formation.[1] (b) Conformationally-accelerated intersystem crossing.[2] (c) Theoretical modelling of energy transfer.[3]

ORAL SESSION 6, LECTURE THEATRE 401-439, 1 DECEMBER, 2023, 12.10 – 12.25 PM

Electrolyte Design and Synthesis for Sodium-Ion Batteries

Darren M. C. Ould,[1] Svetlana Menkin,[1] Holly E. Smith,[1] Clare P. Grey[1] and Dominic S.Wright[1]

[1] *Yusuf Hamied Department of Chemistry, University of Cambridge*

The global drive towards net zero requires suitable energy storage solutions. Lithium-ion batteries (LIBs) currently lead the way in battery technology; however, their ever-increasing demand causes significant problems due to the low abundance and high cost of lithium and cobalt (a key metal in the cathode). Sodium-ion batteries (SIBs) are an attractive alternative that have significant cost and sustainability advantages over LIBs. Unlike lithium, sodium is widely abundant and evenly distributed across the globe. The sustainability of SIBs is further improved as they allow cobalt-free cathodes to be used and the copper current collectors at the anode (used in LIBs) to be replaced by aluminium.[1]

This presentation focuses on the electrolyte for sodium-ion batteries, where the benchmark salt is $NaPF_6$.[1] Although commercial supplies are readily available, due to the hygroscopic nature of $NaPF_6$ they often contain NaF (a hydrolysis product) and are not suitable for battery use. This presentation details the synthesis of battery-grade $NaPF_6$, which unlike other methods does not use toxic HF gas. Instead, our method involves the addition of NH_4PF_6 with sodium metal. This synthesised $NaPF_6$ allows for the exploration of higher concentration electrolyte solutions, where electrochemical advantages are seen.[2] In addition, sodium borates as alternative electrolyte salts will be showcased. These sodium borate salts show higher air stability, give a more stable electrode-electrolyte interface and greater sodium-ion capacity retention than $NaPF_6$.[3]

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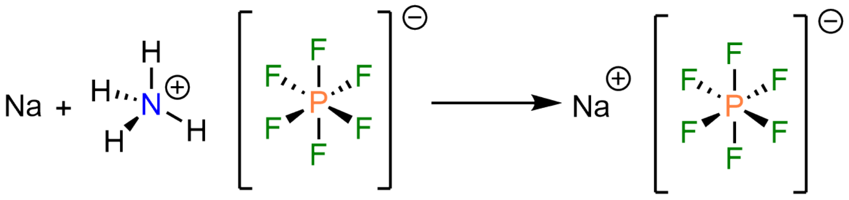
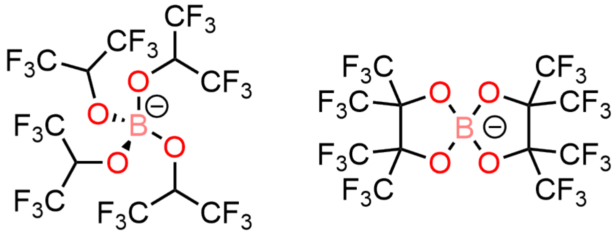


- Synthesis of battery-grade $NaPF_6$
- No HF involved
- Allows for high concentration studies



- Next generation electrolyte salts
- Improved chemical and electrochemical stability

Figure: Overview of $NaPF_6$ synthesis (top) and sodium borate electrolyte salts (bottom).

ORAL SESSION 7, LECTURE THEATRE 401-401, 1 DECEMBER, 2023, 2.00 – 2.20 PM

Regulating Lithium Metal Interfaces to Enhance the Cycle Life of Anode-free Lithium Metal Batteries

Dong Jun Kim[1]

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Anode-free lithium metal batteries (AFLMBs) stand as a highly promising solution for low-cost, high-energy density energy storage systems. By eliminating the conventional graphite anode, AFLMBs become significantly more cost-effective. Despite these advantages, they do come with a few drawbacks, such as the inferior stability of the solid electrolyte interphase layer and the inhomogeneous deposition of lithium during charge and discharge processes, leading to rapid capacity degradation. In this presentation, I will introduce two different coating techniques that offer a viable approach to achieve uniform lithium deposition across the current collector, resulting in densely packed lithium layers. In-situ optical microscopy and Raman mapping have provided conclusive evidence, showcasing that this coating fosters consistent lithium deposition throughout the current collector, leadingto a densely packed and highly stable lithium layer during cycling processes. The results demonstrate the effectiveness of a simple bio-inspired coating, which could remarkably enhance the energy density of anode-free configurations. By enhancing the stability and performance of AFLMBs, our research takes a significant step toward the practical design and realisation of reliable anode-free lithium metal batteries, bringing us closer to a more sustainable and efficient energy storage solution.

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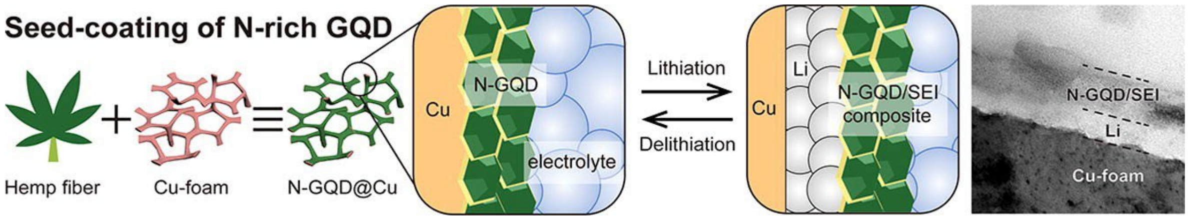

Figure: Schematic illustration of the synthesis process for nitrogen-doped graphene quantum dots anda cross-sectional image of a Li-plated electrode.

ORAL SESSION 7, LECTURE THEATRE 401-401, 1 DECEMBER, 2023, 2.20 – 2.40 PM

Exploring the potential for ionic liquid derived bio-degradable and bio-compatible proton conducting membranes

Patricia Hunt,[1,2] Rebecca Rowe [2]

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[2] *Department of Chemistry, Imperial College London, United Kingdom*

The need to store and convert energy generated through renewable technologies has focused attention on improving, and developing new battery, supercapacitor, solar cell and fuel cell capabilities. Critical to the development of these technologies is the electrolyte. Polymeric electrolytes limit leakage and reduce risks due to flammability or toxicity. Battery and fuel cells polymeric electrolytes are almost exclusively fossil fuel derived and/or non-biodegradable. Wearable electronic devices are of current interest and focus has been on flexible, transparent, bio-compatible electrolytes. Research in polymeric-electrolytes is switching to study renewable, sustainable, bio-derived, bio-compatible and bio-degradable polymers.

There is now interest in considering carboxylic-acid based polymer electrolytes and membranes. However, bio-derived poly-electrolytes have a lower conductivity compared to fossil fuel derived electrolytes. Our focus is poly-anion electrolytes derived from ionic liquid monomers for proton conducting membranes in fuel-cells. Specifically, carboxylate polymers based on polyacrylate anions paired with imidazolium-based cations. The poly-anion and imidazolium ionic nature offers potential new routes to enhance proton conductivity. We have varied the carboxylate alkyl chain and imidazolium functionalisation and obtained an increasein conductivity from 10^{-12} to 10^{-5} S cm^{-1} at 25°C. However, the molecular level characteristics of poly-carboxylate imidazolium anionic-polymer electrolytes are unknown and the mechanismof proton transport has not been elucidated. We have employed DFT calculations; to understand the fundamental inter-ion interactions, rationalise our experimental results and to probe the proton conduction mechanism.

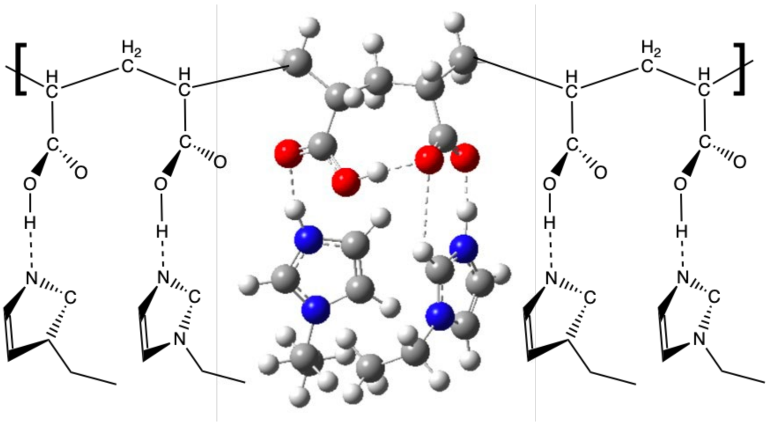

Figure: Optimised model conformer along proton transfer pathway

ORAL SESSION 7, LECTURE THEATRE 401-401, 1 DECEMBER, 2023, 2.40 – 2.55 PM

High-pressure H2 and CO2 Production from Formic Acid

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[2]Doctral Program in Chemistry, Degree Programs in Pure and Applied Sciences, GraduateSchool of Science and Technology, University of Tsukuba

As concern over rapidly escalating energy issues grow, molecular hydrogen (H_2) is being considered one of the most promising clean and renewable energy carriers to bridge the gaps between energy production and consumption. Due to its low volumetric energy density, H_2 is preferably stored physically or chemically in materials termed H2 carrier. Formic acid has gained considerable attention as one of the liquid organic hydrogen carriers due to its beneficial properties such as stability under ambient conditions, biodegradability, and easy handling. Recently, we developed both homogeneous and heterogenous catalysts for the production of high-pressure H_2 and carbon dioxide (CO_2) through the dehydrogenation of formic acid without requiring any mechanical compressing procedures.[1] This method efficiently produces high-pressure gas (CO_2+H_2) over 150 MPa.[2] Even though our system can generate high-pressure gas from formic acid, the resulting gas needs be separated into H_2 and CO_2 for use in fuel cells such as Fuel Cell Vehicles (FCVs). To facilitate effective separation, we further developed the simple method maintaining pressure using gas-liquid phase change under high-pressure conditions (Figure 2). This method enable us to separate95% of H2 gas and 99% of liquid CO2 with 99% of recovery yield in a single step.[3] In this presentation, I will discuss the kinetics of high-pressure gas generation, the related reaction mechanisms, and catalytic deactivation, which could be valuable for industrial applications.

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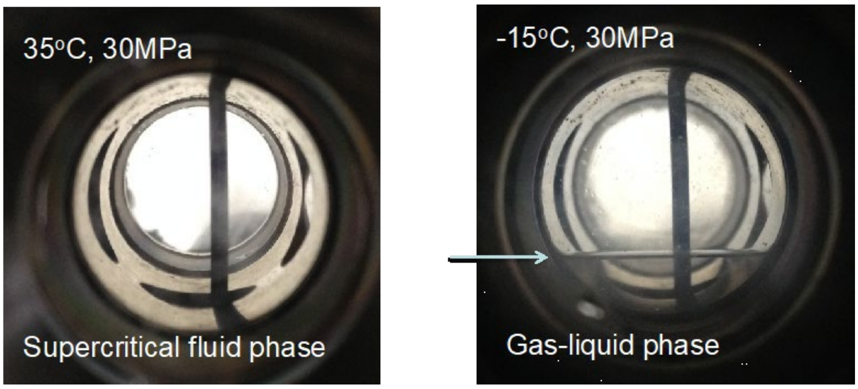

Figure: H_2/CO_2 gas separation from the formic acid dehydrogenation under high-pressure conditions

ORAL SESSION 7, LECTURE THEATRE 401-401, 1 DECEMBER, 2023, 2.55 – 3.10 PM

Poly(3-hexylthiophene)-based Graft Copolymers for Smart Self-transform Novel Transient Electronics

Xin Sun,[1,2] Eddie Wai Chi Chan,[1,2] David Barker,[1,2] Jadranka Travas-Sejdic[1,2*]

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[2]*MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington 6140, New Zealand*

Conducting polymer (CP)-based transient electronics is a new frontier in the electronic materials field. Utilising biodegradable components in electronics to obtain transience is a typical strategy for fabricating environmental-friendly transient electronics. Previous CP- based research focused on blends with biodegradable polymers or block copolymers with biodegradable blocks.[1,2] However, the conductivity of blends or copolymers is generally inferior to pure conducting polymers, partly due to a need for more polymer crystallisation that facilitates charge mobility. Herein, we developed a novel class of transient polymer electronics based on CP graft copolymers, poly(3-hexyl thiophene) (P3HT)-*graft*-gelatin, by covalently attaching relatively short chains of P3HT onto biodegradable gelatin. P3HT crystalline domains were guided to be formed surrounded by gelatine's amorphous domains, allowing interchain charge transfer and therefore contributing to enhanced conductivity of the P3HT-*graft*-gelatin. In the enzymatic degradation experiments, the gelatin backbone was disintegrated, and therefore hydrophobicity of the whole system was changed. The hydrophilic shell of gelatine chains enfolded P3HT, and the degradation components were smartly transformed from thin films to micellar nanoparticles with good biocompatibility. This work opens up the possibility of developing biocompatible and easily metabolised P3HT-based polymer materials for applications in next-generation implantable transient electronics.

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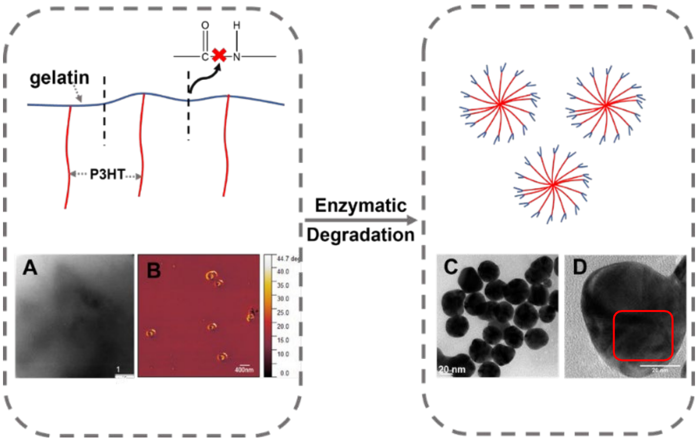

Figure: Scheme of P3HT-*graft*-gelatin before and after enzymatic degradation (blue: gelatin, red: P3HT). A. TEM image of P3HT-*graft*-gelatin in THF and water (v:v=1:1). B. Atomic force microscope (AFM) phase images of P3HT-*graft*-gelatin drop-casted on Mica substrate. C and D are TEM imagesof P3HT-*graft*-gelatin after degradation with the lattice of P3HT forming in the core (marked in the redbox).

ORAL SESSION 7, LECTURE THEATRE 401-439, 1 DECEMBER, 2023, 2.00 – 2.20 PM

Modular assembly of biomimetic catalysts from amphiphilic precursors

Olivia Matich,[1,2] Bhanumathi Bandi,[1,2] Bryan Andres Tiban Anrango,[1,2] Chloe Z.-J. Ren,[1,2]Pablo Solis-Munana,[1,2] Mohinder Maheshbhai Naiya,[1,2] Jack L-Y. Chen,[1,2]

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Cooperative interactions between precisely positioned functional groups in an active site are one of the hallmarks of natural enzymes. Taking this queue from biological systems, chemists have devised numerous strategies for the pre-organization of functional groups to allow the formation of multiple contacts with a bound substrate. Recently, we demonstrated that such cooperative interactions can also be achieved within self-assembled vesicles.[1,2] Inthis talk, we will show how the self-assembly of amphiphilic molecules can be used as a strategy for the screening and optimization of biomimetic enzymes. Unlike conventional approaches that rely on the attachment of key functional groups onto molecular scaffolds or surfaces, the modular assembly of amphiphiles greatly expands the number of catalytic combinations that can be investigated with minimal synthetic effort. Here, we demonstrate the process of optimizing an artificial esterase from amphiphiles that act as a nucleophilic catalyst, an oxyanion hole and a metal ion chelator, to arrive at esterolytic activity that compares favorably to native α-chymotrypsin.

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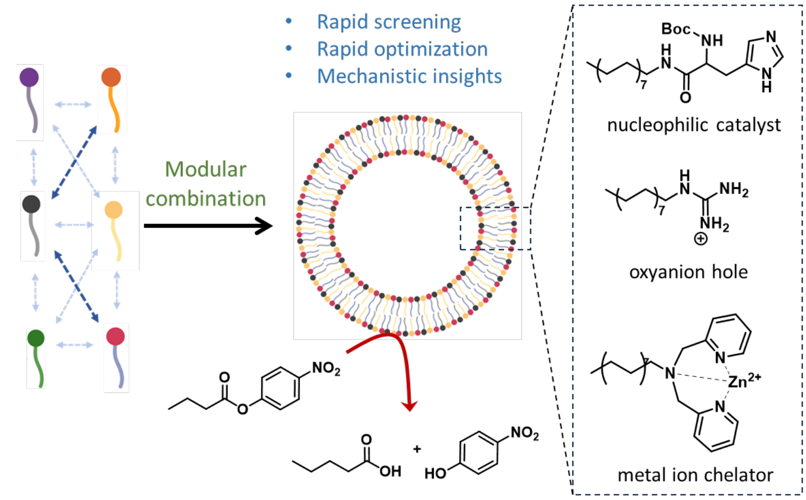

Figure 1. Modular assembly of an artificial esterase

ORAL SESSION 7, LECTURE THEATRE 401-439, 1 DECEMBER, 2023, 2.20 – 2.40 PM

Using TSE as a Route to Sustainable Manufacture

Deborah E. Crawford,[1] Stuart L. James,[2] Aaron S. McCalmont,[2]

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There is a pressing need for new approaches to chemical manufacturing that are more sustainable than conventional solvent-based methods. Twin-Screw Extrusion (TSE), in which reagents are mixed and conveyed along a confined, temperature-controlled barrel by two intermeshing, rotating screws,[1] is emerging as a viable mechanochemical technique in which continuous, solvent-free synthesis, favourable to industrial implementation, can be achieved. Specifically, it has been shown capable of the continuous, kghr^{-1} synthesis of cocrystals[2] and Metal Organic Frameworks (MOFs).[3] TSE has more recently been employed for the solvent-free synthesis of the Active Pharmaceutical Ingredient (API) nitrofurantoin,[4] with a cradle-to-gate Life Cycle Assessment (LCA) highlighting that TSE offers cost, sustainability, and operational advantages over the conventional, solvent-batch system.[5] Furthermore, the facile synthesis and subsequent co-amorphisation of Paracetamol, with citric acid, has been achieved under solvent-free conditions, highlighting the potential of TSE for improving drug bioavailability.

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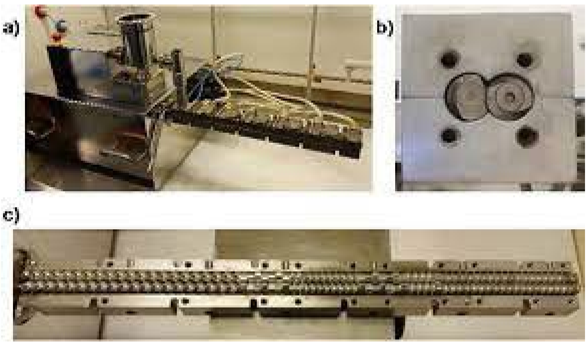

Figure: Twin-screw extruder employed in the continuous, solvent-free synthesis of organic andcoordination compounds.

ORAL SESSION 7, LECTURE THEATRE 401-439, 1 DECEMBER, 2023, 2.40 – 2.55 PM

Remarkable Catalytic Activity of Molybdenum Complexes Bearing 4-[3,5-Bis(trifluoromethyl)phenyl]pyridine-Based PNP- Type Pincer Ligand toward Ammonia Formation

Taichi Mitsumoto,[1] Kazuya Arashiba,[1] Shogo Kuriyama,[1] Yoshiaki Nishibayashi[1]

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The development of sustainable ammonia formation from dinitrogen has been widely studied to use ammonia as an energy carrier toward decarbonization. In some decades, ammonia formation catalyzed by transition metal complexes has been widely studied as an alternative to the Haber-Bosch process, which consumes over 1% of fossil fuel. Recently, we developed molybdenum-catalyzed nitrogen fixation under ambient reaction conditions using samarium diiodide (SmI_2) as a reductant and alcohols or water as cheap proton sources.[1] In this reaction, molybdenum complexes bearing pyridine-based PNP-type pincer ligands were used as effective catalysts. As an extensive study, we have found that the newly designed and prepared molybdenum complex bearing a PNP-type pincer ligand worked as an excellent catalyst toward ammonia formation.[2]

We have investigated the substituent effect at the 4-position of the pyridine ring in the PNP-type pincer ligand toward the reaction of an atmospheric pressure of dinitrogen with SmI_2 and water under ambient reaction conditions. As a result, we confirmed that molybdenum complexes bearing electron-withdrawing groups at the 4-position of the pyridine ring in the PNP-type pincer ligand acted as more effective catalysts. Based on the result of the substituent effect and DFT calculations, we newly designed and prepared a novel molybdenum complex bearing a 4-[3,5-bis(trifluoromethyl)phenyl]pyridine-based PNP-type pincer ligand. The complex worked as an excellent catalyst toward ammonia formation, where up to 3580 equivalents of ammonia were formed based on the catalyst. The catalytic activity was significantly improved by one order of magnitude larger than those observed when using the complex before modification.

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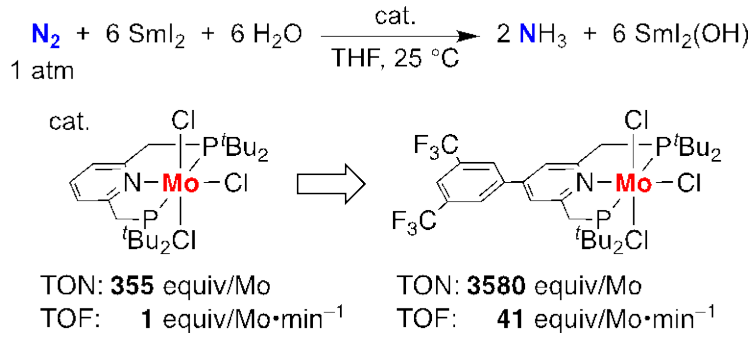

Figure: Catalytic ammonia formation in the presence of molybdenum complexes

ORAL SESSION 7, LECTURE THEATRE 401-439, 1 DECEMBER, 2023, 2.55 – 3.10 PM

Ball Milling as a Scalable Destruction Technology for Toxic 'Forever Chemicals'

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[2]*Environmental Decontamination (NZ) Limited, Auckland, New Zealand.*

Per- and polyfluoroalkyl substances (PFASs) are a class of synthetic chemicals of concern that have been used ubiquitously across industrial and commercial sectors for the last 70 years. PFASs exhibit extreme persistence upon release to the environment and possess physicochemical properties that are resistant to targeted degradation, while also being associated with numerous negative health effects. Treating such pollutants is a highly regulated and complex facet of the hazardous waste industry that considers efficacy, scalability, cost, safety, and treatment time. Ball milling, or mechanochemical destruction (MCD), is a novel treatment technology that exploits the mechanical energy of fast-moving ball bearings in milling vessels to initiate and propagate the mineralisation of PFASs. This technique has been shown to destroy organic contaminants without the need for hazardous oxidizing agents, extreme temperatures, harmful solvents, or high pressures.[1]

In this work, a comprehensive analytical approach was undertaken to determine the fundamental underlying mechanisms of MCD reactions for PFASs spiked onto quartz sand as a grinding auxiliary. Quantitative analysis of ball milled samples revealed high destruction efficiencies ranging from 99.95% to 100% for five different PFAS standards subjected to MCD conditions. Based on the intermediates identified as part of the degradation product analysis, core mechanistic steps have been proposed. Subsequently, the MCD technique was applied to 'real-world' challenges, specifically for the destruction of PFASs in contaminated soil. Upon mechanochemical treatment, the observed destruction was 100% for a wide range of PFASs, demonstrating the capability of the MCD technique to address industrially relevant pollution challenges.

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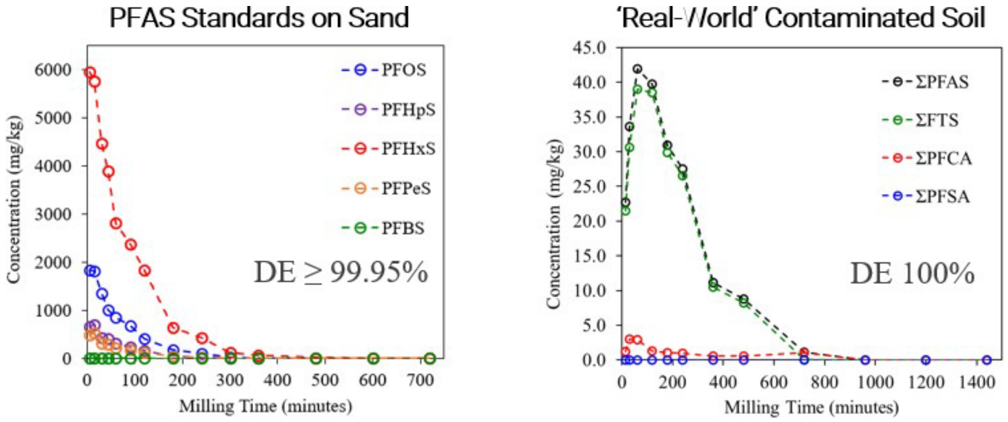

Figure: PFAS destruction observed upon mechanochemical milling. Left: destruction curve of PFASstandards spiked onto quartz sand. Right: destruction curve of PFASs in contaminated soil.

ORAL SESSION 7, LECTURE THEATRE 401-439, 1 DECEMBER, 2023, 3.10 – 3.25 PM

The Origin of the Waterfall Effect: The Earliest Known Example of On-Water Chemistry.

Alexander K. L. Yuen[1], James K Beattie[2] Anthony Masters[1], Thomas maschmeyer[1]

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The waterfall effect describes the separation of charge by splashing at the base of a waterfall. Smaller drops that have a net negative charge are created, while larger drops and/or the bulk maintain overall charge neutrality with a net positive charge. Since it was first described by Lenard (1892) the effect has been confirmed many times, but a molecular explanation has notbeen available. Application of Beattie & co-worker's a fluctuation-correlation model of hydrophobic hydration accounts for the negative charge observed at aqueous interfaces withlow permittivity materials. The negative surface charge observed in the waterfall effect is created by the preferential adsorption of hydroxide ions generated from the autolysis of water. On splashing, shear forces generate small negative drops from the surface, leaving a positive charge on the remaining large fragment. The waterfall effect is a manifestation of the generalphenomenon of the "on water effect": negative charge at the interface between water and hydrophobic surfaces that is created by the preferential adsorption of hydroxide ions.

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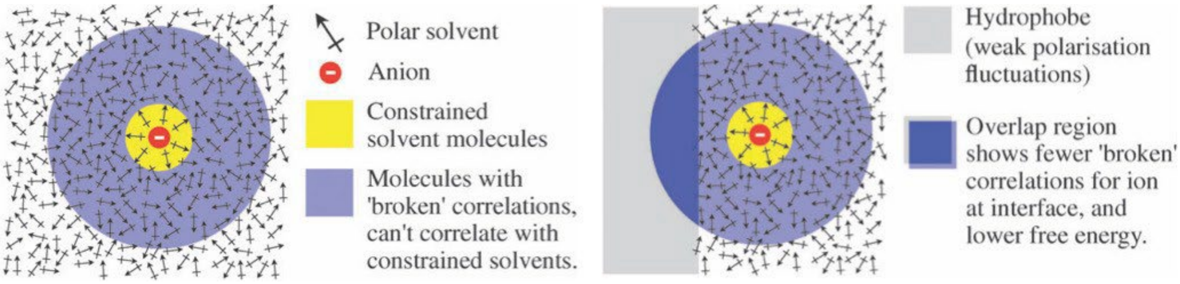

Figure 1: An ion in a polar solvent (*left*) is shown with a solvation shell of molecules that are not so freeas the others to fluctuate (the shaded inner circle represents the constrained solvation sphere). The larger shaded circle represents the range of correlations, and includes those molecules that would be correlated with those in the solvation sphere of the ion, were these inner molecules not constrained bythe ion. The molecules inside the larger shaded circle have their correlations with the ion's hydration sphere 'broken'. When the same ion is close to an interface with a hydrophobe (*right*), the free energy cost of the ion's constrained environment is lower, because there are fewer solvent molecules whose correlations with the hydration sphere are broken by the ion. This is shown by the dark overlap of the correlation sphere with the hydrophobe.

PLENARY SESSION 3, LECTURE THEATRE 401-401, 1 DECEMBER, 2023, 4.00 – 5.00 PM

Sustainable Materials for Energy Storage and Conversion Technologies

Magda Titirici

Imperial College London, Department of Chemical Engineering

This increasing demand of clean energy will need to be met by a combination of existing as well asnew emerging energy sources and technologies. However, this mix of energy sources and new technologies will also affect our environment.

Therefore, when developing novel energy technologies, we always need to also consider the environmental concerns that go hand in hand with modern society's function. This goal cannot be accomplished without developing novel sustainable materials which will be based on clean manufacturing technologies and renewable and abundant resources.

Biomass, in particular waste biomass, which is not in competition with the food chain, represents a suitable platform for sustainable materials production to build novel energy storage and conversion technologies.

In this talk, I will present our latest group research advances in the production of electrodes for flexible supercapacitors from lignin, Na-ion batteries electrodes from cellulose and bioinspired porous carbons for oxygen and biomass electrocatalysis.


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POSTER ABSTRACTS

Session: Thursday 30th November 2023, 5.00 – 7.00 PM, Engineering Building 405 Level 4 Foyer

1. Decarbonylation of Diaryl 1,2-Diketones via Oxidative Addition by a Multifunctional Au−Pd Alloy Nanoparticle Catalyst

Takehiro Matsuyama,[1] Takafumi Yatabe[1], Tomohiro Yabe,[1] Kazuya Yamaguchi[1]

[1]*The University of Tokyo, Tokyo, Japan*

Diaryl ketone is an essential moiety in various fields of chemistry, and various synthetic methods of ketones, including cross-coupling reactions, have been developed to date. A new approach to ketone synthesis via 1,2-diketones has been paid attention to due to the possibility of utilizing various starting materials such as alkynes, alkenes, ketones, and aldehydes. However, reported decarbonylation of 1,2-diketones to ketones mostly dependson a kind of benzilic acid rearrangement utilizing a stoichiometric amount of base and anilines,[1] and a few reports of 1,2-diketone decarbonylation involving oxidative addition demonstrated limited substrate scopes such as aliphatic diketones[2] or alkynyl 1,2- diketones.[3]

In this study, we have developed heterogeneously catalyzed decarbonylation of diaryl 1,2- diketones involving oxidative addition to afford diaryl ketones and CO using a multifunctional CeO_2-supported Au–Pd alloy nanoparticle catalyst (Au−Pd/CeO_2) (Figure).[4] Au−Pd/CeO_2 was confirmed to function as a heterogeneous catalyst by hot filtration and ICP-AES analysis, and the catalyst can be reused. This system demonstrates a wide substrate scopeand functional group tolerance (24 examples). In addition, we also report a tandem reaction starting from benzoins or 1,2-diols to synthesize diaryl ketones using the catalyst via dehydrogenation followed by decarbonylation in the presence of a hydrogen acceptor (17 examples in total). In this presentation, we will discuss the alloy effect and the support effectin detail based on the thorough catalyst characterization, kinetic analysis, and control experiments.

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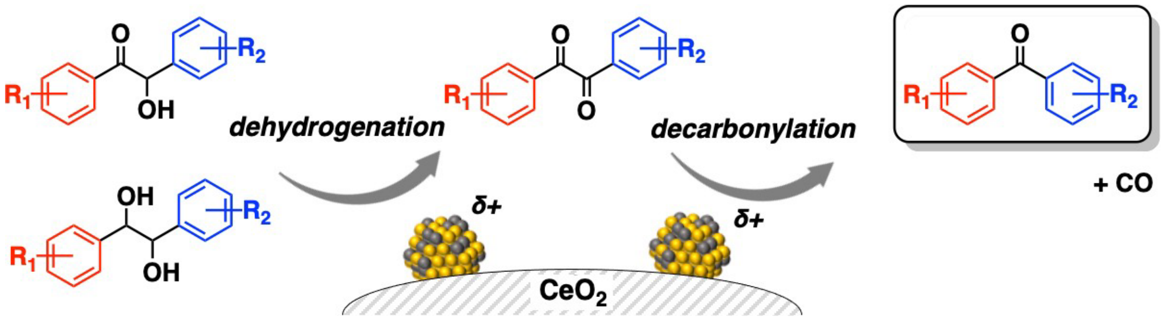

Figure: Diaryl 1,2-diketone decarbonylation to afford diaryl ketones via oxidative addition.

2. Aromatic long chain cations of amphiphilic ionic liquids permeabilise the inner mitochondrial membrane and induce mitochondrial dysfunction at cytotoxic concentrations

Meryem-Nur Duman,[1] Tristan Rawling,[1] Alexander Angeloski[1,2] and Michael S. Johnson[3,4]

[1]School of Mathematical and Physical Sciences, Faculty of Science, University ofTechnology Sydney, Sydney, NSW, 2007, Australia.

[2]National Deuteration Facility, Australian Nuclear Science and Technology Organisation,Lucas Heights, Sydney, NSW, 2232, Australia.

[3]School of Life Sciences, Faculty of Science, University of Technology Sydney, Sydney,NSW, 2007, Australia.

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Ionic liquids (ILs) are used as green alternatives to conventional solvents due to their favourable physicochemical properties. Recent evidence suggests that ILs, and in particular amphiphilic ionic liquids (AmILs), are toxic to humans, plants and animals. Given their high aqueous solubility and chemical stability there is a risk that AmILs could become an environmental pollutant similar to perfluoroalkyl substances (PFASs).[1] Thus, understanding the cellular mechanisms and structural features associated with IL cytotoxicity is important. Current evidence suggests AmILs kill cells by disrupting cellular membranes and/or inducing mitochondrial dysfunction. AmILs share structural features with lipophilic cations, which are known to accumulate in mitochondria in response to the membrane potential across the inner mitochondrial membrane (IMM). Therefore, we hypothesised that AmILs exert their cytotoxic effects by disrupting the IMM, the integrity of which is critical to important cellular processes. Using fluorescence microscopy we show a quinolinium-based AmIL rapidly accumulates in the mitochondria of HeLa cells. In a panel of AmILs we found that AmIL cytotoxicity correlates with their capacity to disrupt lipid bilayers, and that AmILs produce a range of cellular effects consistent with permeabilisation of the IMM at cytotoxic concentrations. AmILs depolarise the IMM, inhibit oxidative phosphorylation and ATP synthesis, and induce ROS formation (Figure 1). These effects were only induced by aromatic AmILs substituted with long (decyl) alkyl chains, as these features promote accumulation in, and permeabilisation of, the IMM.[2] These mechanistic insights help explain the structure–activity relationship governing AmILs cytotoxicity and may be used to rationallydesign AmILs with reduce cytotoxicity.

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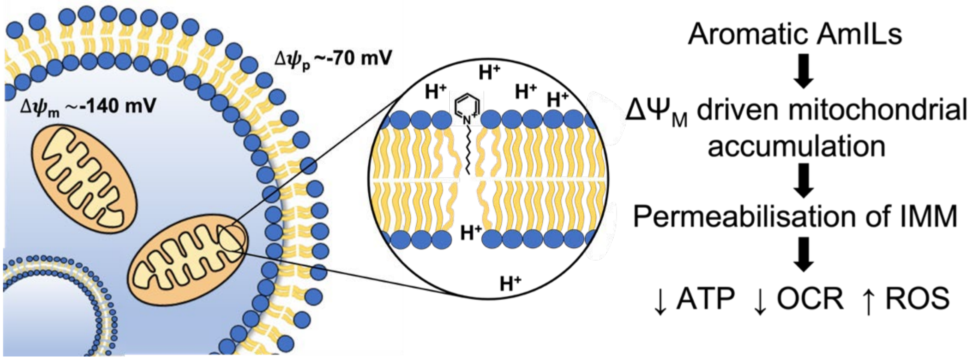

Figure 1: AmILs produce a range of cellular effects consistent with permeabilisation of the IMM atcytotoxic concentrations.

3. Visible Light-Driven Urea Synthesis from CCl4 Promoted by Metal Complex Modified Semiconductor Hybrid Catalyst

Keita Shichijo, Hisashi Shimakoshi

Graduate School of Engineering, Kyushu University

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Development of green and sustainable methodologies for the fine chemical synthesis is highly attractive and much in focus in recent years. Solar energy (visible light) is renewable and clean energy resources having excellent prospects of its utilization in green and sustainable fine chemical synthesis. Thus, visible light-responsive functional photocatalysts have been developed to realize the effective visible light-driven molecular transformations.[1] We have recently developed a visible light-driven hybrid catalyst (B_{12}–Mg^{2+}/TiO_2) composed of a vitamin B_{12} derivatives, which is a bio-derived metal complex, and Mg^{2+} modified TiO_2, which is a visible light-responsive semiconductor photocatalyst.[2] The B_{12}–Mg^{2+}/TiO_2 can effectively produce catalytically active species under visible light ($\lambda \geq 420$ nm) irradiation. Therefore, this hybrid catalyst has a potential to be applied to the visible light-driven fine chemical synthesis. In this paper, we will report a novel visible light-driven fine chemical synthesis catalyzed by the B_{12}–Mg^{2+}/TiO_2 photocatalyst. Specifically, this hybrid catalyst promoted visible light-driven ureas, carbonate esters, and carbamates synthesis from a carbon tetrachloride, CCl_4, in aerobic condition at room temperature. This visible light-driven fine chemical synthesis makes a contribution for the green and sustainable chemistry from two perspectives: utilization of sustainable solar energy and conversion of environmental pollutant, such as CCl_4, into valuable fine chemicals.

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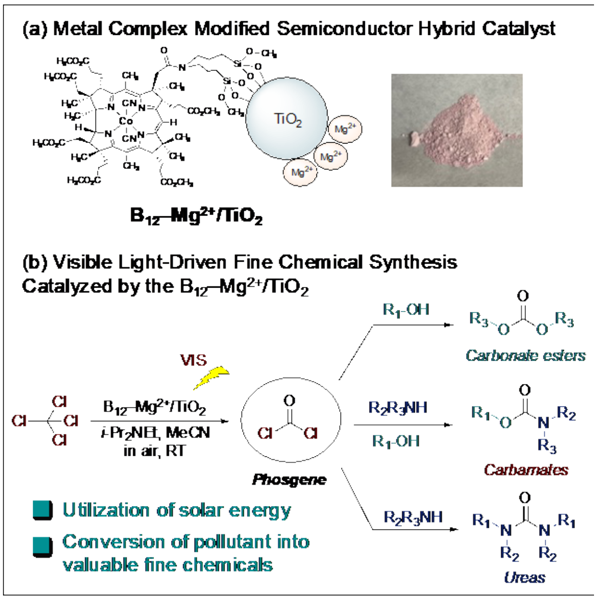

Figure: (a) Hybrid catalyst of B_{12}–Mg^{2+}/TiO_2. (b) Visible light-driven fine chemical synthesis.

4. Formic acid formation from CO2 under non-basic conditions

Seo Ono,[1,2] Ryoichi Kanega,[3] Hajime Kawanami[1,2]

[1]*Doctoral Program in Chemistry, Degree Programs in Pure and Applied Sciences, GraduateSchool of Science and Technology, University of Tsukuba*

[2]*Inderdisciplinary Research Center for Catalytic Chemistry, National Institute of AdvancedIndustrial Science and Technology*

[3]*Reseach Institute for Energy Conservation, National Institute of Advanced IndustrialScience and Technology*

“Free-formic acid” production by CO_2 hydrogenation is a compelling topic, as this reaction requires efficient catalysts and a low-cost process under “non-basic” conditions. However, under non-basic conditions, formic acid (FA) is hardly obtained in water due to the equilibrium between FA and CO_2+H_2. The Cp*Ir-4DABP complex (4DABP; 4,4’-diamino-2,2’-bipyridine) possesses a very high catalytic activity, resulting in the generation of high-pressure gases over 150 MPa from FA aqueous solution during FA dehydrogenation (FADH).1) However, in organic solvents, especially in HFIP (1,1,1,3,3,3-hexafluoro-2-propanol), only a few MPa of gas pressure was achieved in the dehydrogenation process of FA compared to water. This suggests that FA is less active for the dehydrogenation in HFIP solution.

Following these results, we studied the reverse reaction of FADH, that is CO_2 hydrogenation in an organic solvent, and achieved a higher turnover number (TON) with FA using HFIP. CO_2 hydrogenation with HFIP was investigated under various pressure conditions. At 1 MPa (CO_2:H_2=1:1), “free-formic acid” was obtained with a TON of 130.

When CO_2 pressure was increased to 12 MPa, the TON was up to 370. The phase behavior during the reaction was observed with high-pressure view cells. The gas phase and HFIP existed in two phases at a total pressure of 1 MPa, whereas the phase transition to a single supercritical phase occurred at a total pressure of 12.5 MPa. From these results, enhancingthe reaction efficiency can be attributed to the dissolution of all components, catalysts, CO_2, H_2 and HFIP in the supercritical phase.2)

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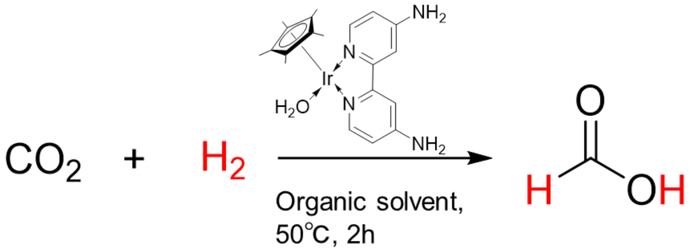

Scheme: The CO_2 hydrogenation in organic solvents under non-basic conditions

5. Hydrophobic pine bark extracts as the starting material for biobased polyesters – Lessons for a bark biorefinery

Regis Risani,[1] Helena Quilter,[1] Suzanne Gallagher,[1] Michael Robertson,[1] Armin Thumm,[1]
Christel Brunschwig[1], Robert Abbel[1]

[1]Scion – The New Zealand Forest Research Institute Ltd., Tītokorangi Drive, Rotorua 3010, New Zealand

About 2.3 million metric tonnes of bark are produced by New Zealand's forestry industry each year, the overwhelming majority from radiata pine (*Pinus radiata*). At current state, most of this biomass constitutes a waste stream. However, studies on other tree species have demonstrated that bark is a rich source for a variety of constituents with significant potential as feedstock for high-value biobased products. The Bark Biorefinery programme explores how New Zealand pine bark can be utilised as a renewable resource for sustainable chemicals and materials. One research aim is dedicated to the extraction, processing, and application of hydrophobic bark components such as waxes and suberin monomers.

We have tested several extraction and fractionation methods and compared them with regards to yield, chemical nature, and functionality of the components. Depending on the extraction process conditions, the hydrophobic fractions are either largely composed of monofunctional long-chain fatty acids and alcohols or contain substantial amounts of difunctional chemicals such as diacids, hydroxyacids and diols. Stoichiometric imbalance (more carboxy than alcohol groups) was identified as a major obstacle towards achieving high molecular weight polymers when the difunctional components where subjected to polycondensation reactions. Comonomer (diol) addition improved yields, solubilities, and molecular weights of the products. Water contact angles of the starting material and the synthesised biopolyesters demonstrated a strong improvement in hydrophobic properties upon polymerisation. We are currently investigating whether these materials have future applications as biobased alternatives to fossil-derived water-repellent coatings.

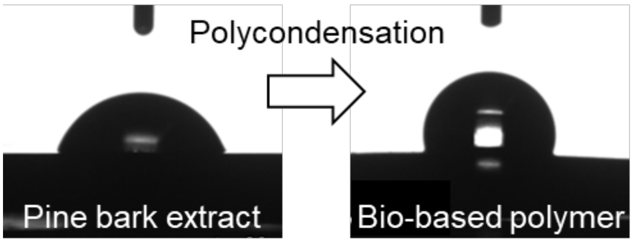

Figure: Water contact angles on pine bark extract starting material (left) and the resulting product after polycondensation (right).

6. Heterogeneously Catalyzed Selective Acceptorless Dehydrogenative Aromatization to Primary Anilines from Cyclohexanones and Ammonia

Hui Li,[1] Takafumi Yatabe,[1] Satoshi Takayama,[1] Kazuya Yamaguchi[1]

[1]*School of Engineering, The University of Tokyo*

Primary anilines are important basic chemicals widely utilized in diverse fields such as organic synthesis, pharmaceuticals, agrochemicals, dyes, electronic materials, polymers, and other industrial chemicals. These relevant compounds are conventionally prepared via classical nitration of arenes followed by reduction of nitrobenzenes; however, this multistep process requires a large amount of acids and cannot directly utilize NH_3 as the nitrogen source. Recently, we developed a selective synthesis of primary anilines via dehydrogenative aromatization from cyclohexanones using NH_3 as the nitrogen source in the presence of a supported Pd nanoparticle catalyst.[1] However, this method requires a stoichiometric amount of styrene as the hydrogen acceptor to avoid undesirable conversion of primary anilines to secondary anilines, which occurs preferentially via reductive *N*- alkylation with cyclohexanones or cyclohexanimine intermediates. Although we also reportednew hydrogen acceptor-free synthesis methods for primary anilines from cyclohexanones, using hydroxylamine or hydrazine as the nitrogen source was indispensable to achieve high efficiency and selectivity.[2,3] Herein, we developed a highly selective synthesis of primary anilines from cyclohexanones and NH_3 via efficient acceptorless dehydrogenative aromatization heterogeneously catalyzed by an $Mg(OH)_2$-supported Pd nanoparticle catalyst in which $Mg(OH)_2$ species are also deposited on the Pd surface ($Pd@Mg(OH)_2$).[4] The basic sites of the $Mg(OH)_2$ support effectively accelerate the acceptorless dehydrogenative aromatization via concerted catalysis, suppressing the formation of secondary amine byproducts. In addition, the deposition of $Mg(OH)_2$ species inhibits the adsorption of cyclohexanones on the Pd nanoparticles to suppress phenol formation, achieving the desired primary anilines with high selectivity.

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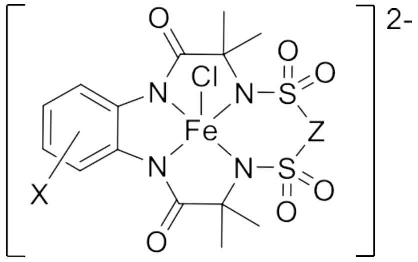
7. New water-soluble iron oxidation catalysts based on the “TAML” macrocyclic core for water purification: Enhanced catalysis with optimal activity at pH 7

Yongjian Chen[1], L. James Wright[1]

[1]*School of Chemical Sciences, University of Auckland, New Zealand*

In the 1980s, Prof T. J. Collins and his group introduced macrocyclic iron complexes(“Fe-TAMLs”) as oxidation catalysts that are capable of removing organic micro pollutants, including endocrine-disrupting compounds (EDCs), from large quantities of water.[1] Fe-TAMLs can be activated by H_2O_2, with the Fe(III) centre of the complex being oxidized to a very reactive Fe(V) oxo intermediate. This is capable of rapidly oxidizing many organic pollutants that are present in low concentrations in water. The latest generation of Fe-TAMLs (“New-TAMLs”), which incorporate two deprotonated carboxamide and two deprotonated sulfonamide donor groups (see Fig 1), exhibit significantly enhanced rates of oxidation (15-20 times faster) compared to the initial Fe-TAMLs.[2] However, they also undergo self-oxidation at a faster rate and the optimal pH range for operation remains restricted to ca. pH 9 or above, which hinders their practical application.



"Head region" "Tail region"
(X = H, NO_2; Z = CH_2, CMeH)

Figure 1. New-TAMLs

By making rational alterations to the both the aromatic ring in the “head region” of the New-TAML macrocycle and bridging group “Z” in the “tail region” we have synthesized a series of analogues that have equally high oxidation rates but operate at pH 7 and undergo much slower self-oxidation. The changes we have made were designed to modify the electronic properties of the donor groups as well as alter the overall charge of the complex. Details of the new complexes, including kinetic measurements of their catalytic oxidation of organic substrates will be presented.

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8. Toxicity of nanoparticles: Surface charge

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The mechanisms, by which nanoparticles interact with biological structures as well as their biological impacts and hazards remain insufficiently understood. Due to the large surface to volume ratio of nanoparticles, their surface chemistry is crucial for nanoparticle stability and solubility in biological media as well as for their biocompatibility and biodistribution. Bulk polystyrene does not degrade in the cellular environment and exhibits no short-term cytotoxicity. Therefore, we have exploited polystyrene nanoparticles as a convenient chemical platform to study biological effects of positively and negatively charged nanoparticles. Carboxyl- (PS-COOH) and amino-functionalized (PS-NH2) nanoparticles were prepared by free-radical copolymerization in a direct (oil in water) miniemulsion system. We show that surface functionalization of polystyrene nanoparticles with amino groups (PS-NH$_2$), but not with carboxyl groups (PS-COOH), induced G$_2$ cell-cycle arrest and inhibition of proliferation in three myeloid leukemia cell lines. Besides, PS-NH$_2$ inhibited angiogenesis and proliferation of leukemia xenografts. At the molecular level, PS-NH$_2$ inhibited, whereas PS-COOH activated mTOR signaling in leukemia cells. Both types of particles rapidly induced autophagy in leukemia cells. Yet, only in PS-NH$_2$–treated cells, acidic vesicular organelles exhibited elevated pH and impaired processing of procathepsin B. Moreover, solely in PS-NH$_2$-treated cells, autophagy was followed by permeabilization of acidic vesicular organelles and inductionof apoptosis. These data indicate that functionalized nanoparticles can be used to control activation of mTOR signaling pathways, to influence proliferation and viability of malignant cells, and to predict their environmental toxicity.

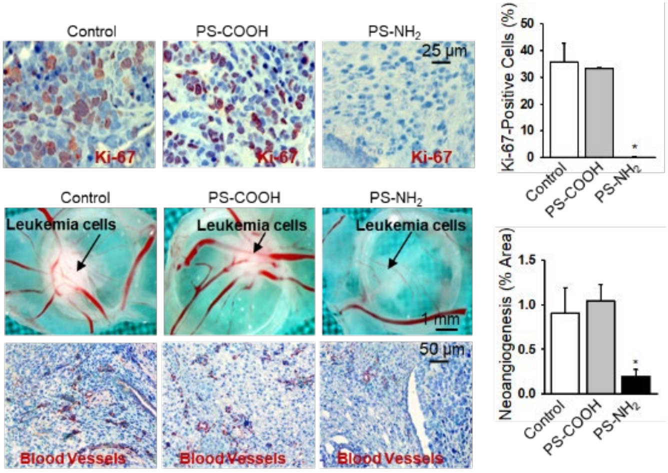

Figure: PS-NH$_2$ nanoparticle are toxic to leukemia xenografts.

9. Bark to the Future: Examining the Selectivity and Efficiency of Pinus radiata bark extractions using ionic liquids

Alice Loretto[1], Lisa Pilkington[1], Cameron Weber[1]

[1]*School of Chemical Sciences, University of Auckland, Auckland 1010, New Zealand*

It is in the world's best interest to find a way to produce chemicals from renewable sources as opposed to finite petroleum-based sources. Biomass-based chemical feedstocks are greener alternatives that are widely available and come from renewable sources.[1] While traditionally bark waste is often burnt on-site or made into wood pellets, paper and other low-value products, it contains many different compounds such as cellulose, hemicellulose, lignin, and suberin, making it a promising renewable source for chemicals.[2,3] If extraction of these components were possible, this would allow for the sourcing of high-value renewable biomass-based products from an otherwise waste material.

Bark extraction typically requires hazardous volatile organic compounds as solvents. Recently, other, more environmentally friendly solvents, such as ionic liquids have been successfully used to extract suberin and other compounds in various tree barks.[4,5] Very little research, however, has explored the use of ionic liquids to extract *Pinus radiata* bark, the most widely-produced variety of bark in New Zealand.

This project aimed to investigate the use of ionic liquids to extract key components from the bark of *Pinus radiata*. This was achieved by the extraction of bark using various ionic liquidsand a range of conditions, followed by IR analysis of the extracts to analyse their chemical composition. Chemometric techniques were employed to identify the optimal ionic liquid(s) and extraction conditions to isolate the components of interest and explore the nature of this selectivity. The results of this investigation will be presented.

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10. A High Performance Supercapattery, Based on a Redox-Active 2D Tetrathiafulvalene-Copper MOF

Jie Dai, Qin-Yu Zhu, Zhi-Ruo Zhang

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Metal-organic frameworks (MOFs) have attracted noticeable attention as promising candidates for green energy storage.[1,2] However, the lack of electrical conductivity and the weak stability of most MOFs result in poor electrochemical performances. Here, a tetrathiafulvalene (TTF)-based complex, formulated as $[(CuCN)_2(TTF(py)_4)]$ (**1**) ($TTF(py)_4$ = tetra(4-pyridyl)-TTF), is assembled by in situ generation of coordinated CN^- from a nontoxic source. Single-crystal X-ray diffraction analysis reveals that compound **1** possesses a two- dimensional layered planar structure, which is further stacked in parallel to form a three- dimensional supramolecular framework. The planar coordination environment of **1** is the firstexample of a TTF-based MOF. Attributed to the unique structure and redox TTF ligand, the electrical conductivity of **1** is significantly increased by five orders of magnitude upon iodine treatment. The iodine-treated **1** (**1**-ox) electrode displays typical battery-type behavior through electrochemical characterizations. The supercapattery based on the **1**-ox positrode and AC negatrode presents a high specific capacity of 266.5 C g^{-1} at a specific current of 1 A g^{-1} with a remarkable specific energy of 62.9 Wh kg^{-1} at a specific power of 1.1 KW kg^{-1}. The excellent electrochemical performance of **1**-ox is one of the best among those reported supercapatteries, demonstrating a new strategy for developing MOF-based electrode materials.

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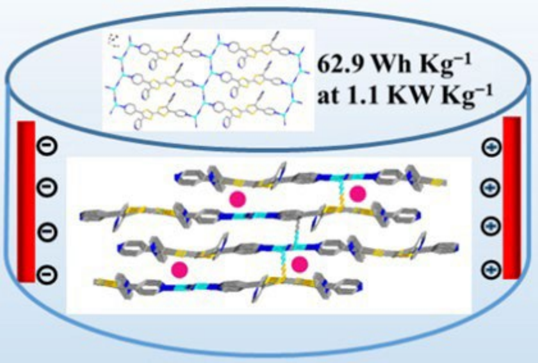

Figure: A redox-active 2D TTF-Cu MOF oxidized by iodine exhibits an enhancement of electrical conductivity and a high specific energy.

11. Nanobubble Generator for Green and Sustainable Agricultural and Aquaculture Applications

Maddodi B S,[1] Amith Kapur,[2] Ananth Kapur,[3] Raghu Bharadwaj R,[4]

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[2]*Manipal Academy of Higher Education Manipal (MAHE) INDIA*

In response to the growing demand for green, sustainable and efficient solutions in agricultural and aquaculture industries, we present a novel nanobubble generator with a patent-worthy design. Nanobubbles, which are ultrafine bubbles with diameters on the nanometer scale, hold tremendous potential in enhancing various processes crucial to the productivity and green environmental sustainability of these sectors. The proposed nanobubble generator leverages cutting-edge nanotechnology and innovative engineering principles to produce a stable and high-density stream of nanobubbles. Our design ensures a consistent nanobubble size distribution, with diameters typically ranging from tens to hundreds of nanometers. The implementation of our nanobubble generator in green and sustainable agricultural spaces promises to revolutionize irrigation practices. Nanobubbles have shown remarkable capabilities in improving water infiltration, soil oxygenation, and nutrient uptake, leading to higher crop yields and reduced water consumption. For aquaculture applications, the nanobubble generator holds immense potential in promoting thehealth and growth of aquatic species. The tiny bubbles carry dissolved oxygen efficiently, alleviating oxygen deficiencies in densely stocked aquaculture systems. Our nanobubble generator design not only presents a ground-breaking technological advancement but also addresses critical environmental challenges faced by these industries Our patentable nanobubble generator has the potential to revolutionize green sustainable agricultural and aquaculture industries by significantly improving productivity, resource efficiency, and ecological sustainability.

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Figure: Nano bubble generator from Neer Shakti Private Limited ®

12. Isolation and characterization of novel naturally occurring sophorolipid glycerides

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Sophorolipids (SL) are promising glycolipid biosurfactants as they are readily produced and functional. Lactonic (LSL) and acidic SL (ASL) are well-known. Here, we used chromatography and suitable solvent systems to find and characterize novel, naturally occurring sophorolipid-glyceride derivatives (SLG) from a *Starmerella bombicola* product[1]. The SL-tri-glyceride and -di-glyceride are highly water soluble; they are more bulky and havea higher molecular weight than typical SL. Furthermore, the surface tension of the purified tri- and di-glyceride aqueous solutions decreases to approximately 40 mN/m, similar to thatof conventional ASL. The tri-glyceride of the two sophorolipids and a fatty acid is more lipophilic, with oily properties and little surface activity. These SLG are the third-most abundant component after the well-known SL in *S. bombicola* products (LSL:ASL:SLG component ratio in our samples was 49.2:33.5:17.3), and synergistic effects are expected when these sophorolipids are mixed.

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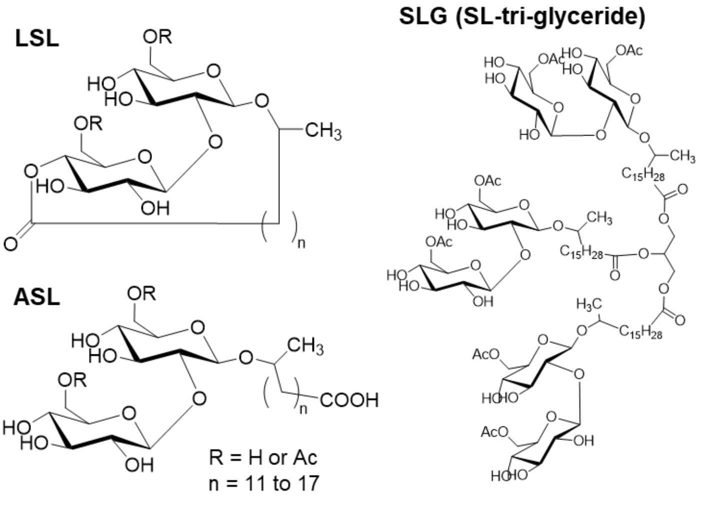

Figure: Chemical structures of sophorolipid derivatives

13. Crystallinity-controlled poly(L-lactic acid) for its enhanced home-compostability by blending with amorphous polymers

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Poly(lactic acid) (PLLA) has many desirable properties as a biodegradable polymer, but its limitations in terms of home compostability have prompted research into ways to improve its biodegradability. One approach that has shown promise is blending PLLA with amorphous polymers, which can interfere with PLLA crystallization and increase its accessibility to microorganisms in the compost. Our study focuses on the blending of PLLA with an amorphous polymer and its impact on the biodegradability of the resulting material under home compost conditions. We found that the microphase separation of the two polymers creates microfluidic channels by the amorphous polymer, which helps to increase the surface area accessible to microorganisms in the compost, facilitating biodegradation of both polymers. Additionally, the low molecular weight acids generated from amorphous polymer can contribute to the auto-catalytic effect, further promoting biodegradation. Our study demonstrates that the PLLA blends have the potential to improve its biodegradability and widen its range of applications.

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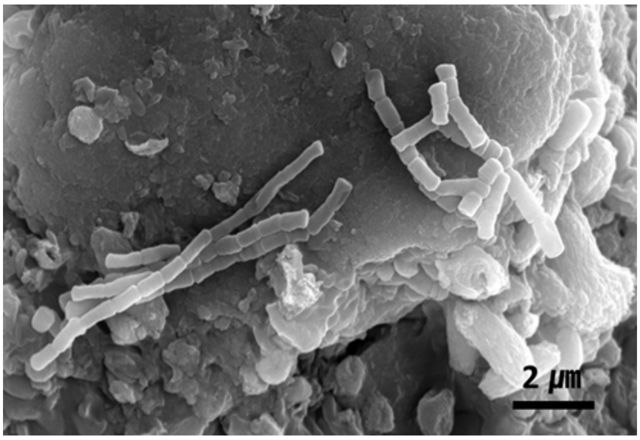

Figure 1. Scanning electron microscopy image of the biodegraded polymer surface by *Bacillussubtilis*.

14. Lignocellulose Nanofibres for Biodegradable Plastic Applications in Agriculture

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Cellulose nanofibres (CNFs) are ultrathin cellulose fibres with diameters in the nanoscale that can be produced by mechanical or chemical treatment of lignocellulosic biomass. CNFs can produce high-performing hydrogels and films with competitive properties, so are quickly emerging as renewable platform materials for sustainable plastic replacements for a wide array of applications. However, the application of CNFs in agriculture is limited by their rapidbiodegradation in ideal soils (>90% in 42 days). To improve their viability for agricultural applications, we investigated the effect of incorporating lignin, a natural antimicrobial polyphenol, to modulate the biodegradation rate of cellulose nanofibres.

Lignin-containing cellulose nanofibres (LCNFs) with varying lignin contents (35%, 26%, and 20%) were synthesised by green mechanochemical treatment of softwood thermomechanical pulp (Pinus Radiata) with a choline chloride-urea deep eutectic solvent. These were incubated in soil at 23℃ and 50% RH for one month to establish the effect of lignin on microbial activity and carbohydrate degradation. Radish and cress seeds were germinated on the LCNFs to determine any impacts on seed germination.

Changing the lignin concentration from 20% to 35% decreased the biodegradation rate from 20.8% $14d^{-1}$ to 5.7% $14d^{-1}$. This result correlated with CO_2 emissions decreasing from 0.110 g/m^2d to 0.0915 g/m^2d for the same treatments. The LCNFs demonstrated no negative effects on soil microbial activity, and no statistically significant difference occurred between mean times to germinate for all treatments of both cress and radish seed germination. This contributes to enabling the use of LCNFs for sustainable plastic replacements in agriculture.

15. The potential of halloysite application for soil remediation

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The presence of heavy metal ions in soil moderates plant growth and inhibits natural processes in the rhizosphere by disruption of the chlorophyll synthesis [1]. An application of widely abounded, low-cost sorption material can reduce the heavy metal content and increase the valuable microelements presence [2]. The halloysite clay mineral mined in Dunino deposit (Poland) was analysed towards surface morphology (SEM) and elements content (mineralization/ICP). Cd(II) and Cu(II) sorption tests were carried out under batch conditions. The metal ion's impregnated material was used for the germination test with the cucumber seeds. Isomorphous substitution of Si^{4+} by Al^{3+} in surface tetrahedral sheets givessmall negative charge of siloxane faces and is responsible for ion exchange. These are so- called permanent active sites with a pH independent charge. Though, halloysite has low sorption capacity (up to a few mg/g), the active sites are randomly distributed on the material surface and easily available for sorption/desorption process (the sorption kinetics was established in a few minutes). In the contrary, the alumina faces and the crystal edges have pH-dependent variable active sites caused by protonation and deprotonation of the silanol and aluminol hydroxyl groups. Their availability for sorption was confirmed by increase of sorption efficiency with decreasing the halloysite particle size. The identified high content of Mg is especially valuable since it is essential micronutrient for plant growth. The germinated test confirmed the halloysite biostimulator effect on the cucumber seeds growth up.

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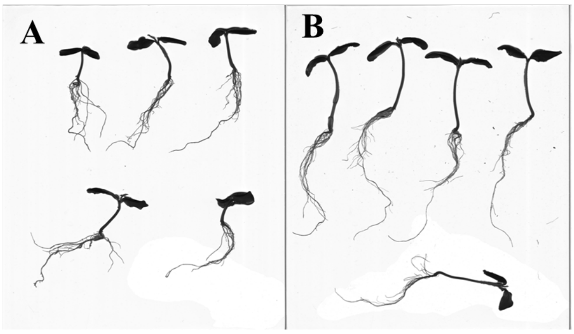

Figure: A comparison of sprouts without applied halloysite (A) and sprouts with a dose of 2.0 g perPetri dish (B).

16. Cr(III) sorption on modified PLA filament

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The development of 3D printing technology in recent years is growing rapidly, especially in the food, medical and technology industries. One of the most popular materials used in 3D printing is lactic acid polymer (PLA) that can be obtained from food or agricultural waste. Regrettably, there are no available functional groups in the PLA structure allowing for heavy metal ions binding [1].

The main objective of this study was to modify the PLA surface by hydrolyzing ester bonding in order to provide it with sorption ability for Cr(III) ions. Influence of modificators' (NaOH and NH_3) concentration and contact time was analysed by using the Box-Behnken Method (Statistica). The effectiveness of carboxylic and hydroxy groups incorporation was evaluatedby ATR-FTIR technique (Vertex 70v, Brucker, USA). The modified PLA was able to uptake Cr(III) with efficiency (qmax) up to 0.467 mmol/g at pH 3.5-4.0 (mechanical shaker, PSU-20i Biosan, 70 rpm). Rapid sorption kinetics follows the II-order pseudo-reaction model.

The proposed modification method of PLA surface creates opportunity for utilization of PLA filaments as a sorption material for heavy metal uptake. So far, the PLA residue is not recycled or used in an alternative way. The further research will focus on printing of 3D filtersfrom modified PLA.

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17. Strategies for creating silica aerogel blanket composites for wide-range thermal insulation applications

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Silica aerogel is a nanoporous solid and the best thermal insulatior to date. However, the potential applications of this lightweight material have been hindered by its inherent fragibilityand brittleness resulting from its ultra-porous nature. The most widely applied form of silica aerogel is found in fiber-reinforced aerogel blankets, but it has the potential to generate dust when handled. In this study, flexible and dust-free silica aerogel blankets were successfully fabricated by laminating or coating thin aerogel blanket sheets. The proper selection of laminating or coating materials allowed for control of the physicochemical properties of the resulting aerogel blanket product as needed. These products can be highly flexible, easily shaped, nonflammable, and even waterproof/breathable. A low thermal conductivity of less than 10 mW/m-K could be achieved by applying a vacuum during lamination. The thermal conductivity of waterproof/breathable resin/fiber laminated aerogel blanket was less than 20 mW/m-K. Multi-layer laminated aerogel blankets can be used for both military and civilian applications, such as boot insoles, outdoor jackets, sleeping mats, and multi-purposeponchos. In this study, we introduce different strategies for making silica aerogel blanket composites.

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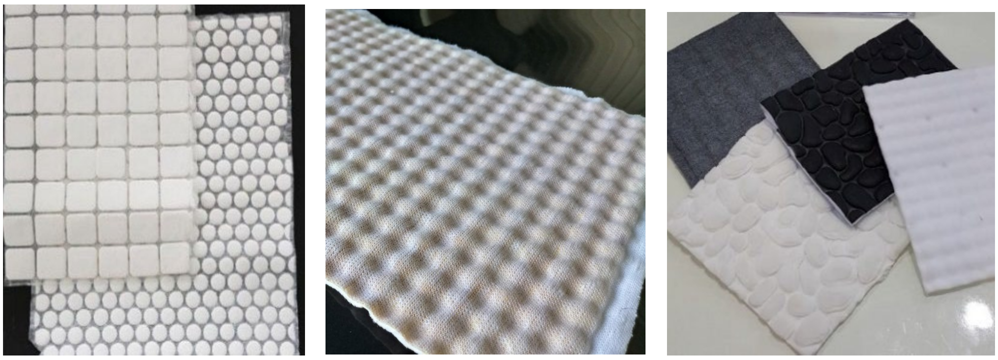

Figure: Various types of multi-layer laminated aerogel blankets

18. Oxidatively Doped Tetrathiafulvalene-Based MOFs for Supercapattery with High Specific Energy

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The growing demands for powerful and sustainable energy sources continuously promote the development of alternative renewable energy source devices.[1,2] In this work, we report the application of oxidatively doped tetrathiafulvalene (TTF)-based MOFs for high performance electrodes in supercapatteries. Two isostructural MOFs, formulated as [M(py- TTF-py)(BPDC)]·$2H_2O$ (M = Ni^{II} (**1**), Zn^{II} (**2**); py-TTF-py = 2,6-bis(4'-pyridyl)TTF; H_2BPDC = biphenyl-4,4'-dicarboxylic acid), are crystallographically characterized. The two MOFs possess a three-dimensional 8-fold interpenetrating diamond-like topology, which is the firstexample for TTF-based dual-ligand MOFs. Upon iodine treatment, MOFs **1** and **2** are converted into oxidatively doped **1**-ox and **2**-ox. The electrical conductivity of **1**-ox and **2**-ox is significantly increased by six~seven orders of magnitude and the specific capacities reach 833.2 and 828.3 C g^{-1} at a specific current of 1 A g^{-1} for **1**-ox and **2**-ox, respectively. When used as a battery-type positrode to assemble supercapattery, the AC‖**1**-ox and AC‖**2**-ox present an energy density of 90.3 and 83.0 Wh kg^{-1} at a power density of 1.18 KW kg^{-1} and great cycling stability with 82% of original capacity and 92% columbic efficiency retention after 10000 cycles. *Ex situ* characterizations illustrate the ligand-dominated mechanism in the charge/discharge processes. The excellent electrochemical performances of **1**-ox and **2**-ox illustrate that the construction of unique highly dense and robust structures of MOFs followed by post-synthetic oxidative doping is an effective approach to fabricating MOF-based electrode materials.

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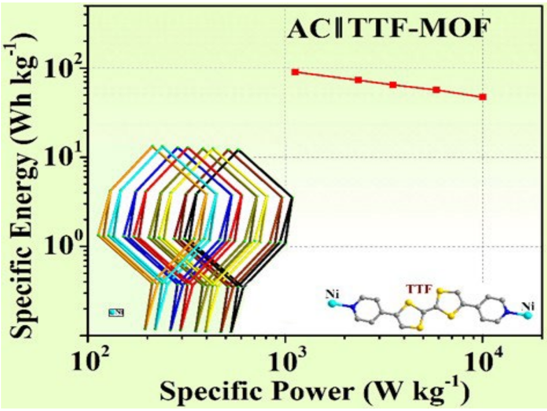

Figure: 3D 8-fold interpenetrating dia-like TTF-based MOFs are synthesized, showing an enhancedconductivity, boosted specific capacity and high specific energy of the supercapattery.

19. Nucleofugality in ionic liquids

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Ionic liquids are promising alternatives to molecular solvents for preparative chemistry.[1] They have been shown to affect the reaction outcomes (*e.g.* rates of reaction) of a range of organic processes.[2] These effects are dependent on the proportion of ionic liquid in solutionand the nature of the ions present, both of which determine the microscopic interactions between the solvent and species along the reaction coordinate.[3]

While a range of reaction outcomes might be qualitatively predicted, they remain difficult to quantify. To overcome this, we have been examining the nucleofugality, a quantitative reaction parameter evaluating the leaving group ability,[4] of a series nucleofuges in mixtures containing ionic liquids.

The work presented here investigates the effects of ionic liquids on the nucleofugality of bromide (Figure 1). These data will be compared to that of the chloride in the correspondingionic liquids,[5] which have been shown to quantitatively predict reaction outcome.[6] This work expands our understanding of solvent effects in ionic liquids and is integral to developing a quantitative predictive framework for the rational selection of ionic liquids in preparative chemistry.

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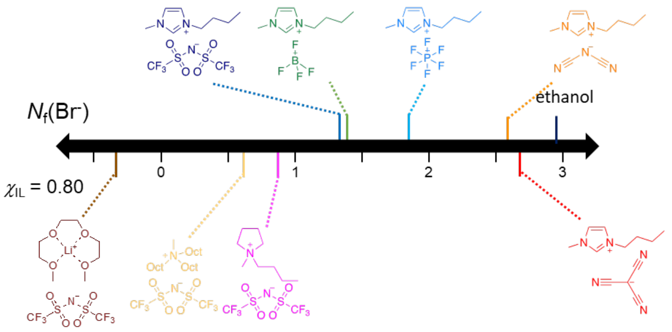

Figure 1. The nucleofugality of bromide in ethanol and each of a series of ionic liquids (χ_{IL} = 0.8).

20. Switchable Solvents for Extraction processes using the bark of Pinus Radiata

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Pinus radiata is the dominant species of tree in the New Zealand forestry industry with 38.3 million m^3 of *Pinus radiata* trees harvested annually. Bark is removed before these trees are processed into logs due to the barks high lignin/polyphenol content causing difficulties in wood processing.[1] The bark waste is currently burnt to provide energy and heat or used as garden mulch despite its potential as a source of biorenewable chemicals such as waxes and polyphenols.

In this work, Switchable Hydrophilicity Solvents (SHSs) which are secondary or tertiary amines that can reversibly switch between hydrophobic and hydrophilic forms are used to carry out extractions from *Pinus radiata* bark.[2] CO_2 at atmospheric pressure is used to trigger the transformation to the hydrophilic form by protonated the SHS. The removal of CO_2 by heating or the addition of an inert gas causes the SHS to switch back to its hydrophobic form.

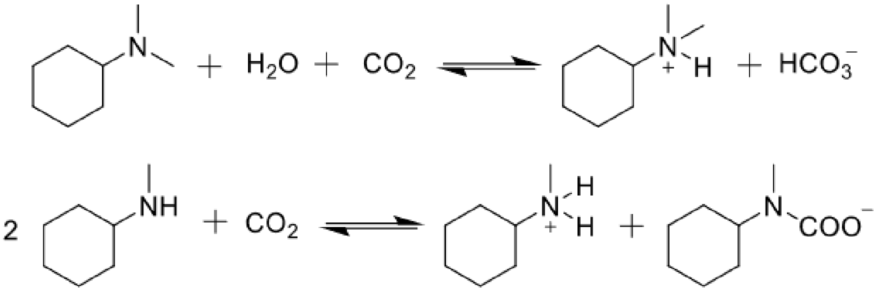

Figure 1: DMCHA and MCHA reacting reversibly with CO_2 to form the hydrophilic switchable solvent.

Extractions from *Pinus raduata* bark were done using N,N-dimethyl-cyclohexylamine (DMCHA) and N-methyl-cyclohexylamine (MCHA) SHSs in both their hydrophobic and protonated forms (Figure 1). This presentation will outline the effect of SHS selection on the selectivity of extractions using both hydrophobic and protonated forms of the SHS. Techniques using GC-MS, GPC, ion chormatography and solid state NMR were used to characterise the extracts and results from these analysis will be presented.

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21. High-pressure hydrogen generation from formic acid using polymer immobilized catalysts.

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The rise in atmospheric CO_2 concentrations and the resulting global average temperatures increase are widely recognized as serious issues. Given this situation, there's an urgent need to transition to hydrogen energy systems to effectively reduce CO_2 emissions. Although hydrogen has a high energy density per weight, its low energy density per volume presents challenges for efficient transportation. Specifically, gaseous hydrogen's extremely low density (0.052 kg/m^3) necessitates compression for storage, but potential energy loss during the compression process remains a major concern. Therefore, we need ahydrogen carrier that can store and transport hydrogen efficiently. We have been proposing the use of formic acid (FA) as a hydrogen carrier. [1] [2] FA not only has a high hydrogen storage capacity (53 kg/m^3, 4.3 wt%), but also offers several advantages, such as high stability, low toxicity, low flammability, and ease of storage and handling.

Recently, we reported the efficient homogeneous Ir catalysts for formic acid dehydrogenation (FADH), [1] [3] [4] and these catalysts enabled the production of high-pressure hydrogen gas above 150 MPa at 80℃. For the practical use of FADH, it is necessary to immobilize these catalysts to ensure the catalyst recyclability and facilitate flow-type continuous hydrogen production. Herein, we synthesized the Ir-based catalysts immobilizedon functional polymers and evaluated these catalytic properties for FADH activity and durability over extended reaction time. Furthermore, we carried out high-pressure hydrogengeneration reactions using these immobilized catalysts.

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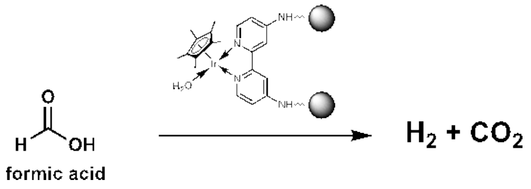

Scheme formic acid dehydrogenation in the presence of Iridium immobilized catalyst

22. Investigating Selectivity in Copper-Catalyzed Phosphoramidate Synthesis using Ionic Liquid Solvents

Luke Park,[1,2] Dr. Cameron Weber,[1,2] Dr. Erin Leitao[1,2]

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Traditionally phosphoramidates have been synthesized by the nucleophilic substitution of chlorophosphonates with amides in the presence of a strong base such as *n*-butyllithium.[1] Recent methods involve aerobic oxidative dehydrocoupling, where phosphites interact with a copper(II) bromide catalyst to produce a halogenated phosphite and copper(I) bromide.[2] Thereduced copper(I) is re-oxidised by air, thus completing a catalytic cycle. The aerobic oxidative dehydrocoupling reaction was examined using ionic liquids as alternative solvents in an effort to explore their kinetic and thermodynamic effects on the reaction. Conditions were also explored using different copper catalysts, as studies in literature have indicated an anion effect on the aerobic oxidation of amines where selectivity between imine and nitrile products could be controlled.[3] $[C_4C_1im][Me_2PO_4]$, $[C_4C_1im][OAc]$, and $[C_4C_1im][NTf_2]$ were used as ionic liquid solvents and compared to ethyl acetate (EtOAc), the most commonly used solvent for this transformation. Copper catalysts included $CuBr_2$, $Cu(OAc)_2$, $CuCl_2$, and $Cu(OTf)_2$. This presentation will outline the effect of the aforementioned ionic liquids and copper catalysts on the selectivity of the phosphoramidate and imine products discussing the effects and mechanisms underlying the changes observed.

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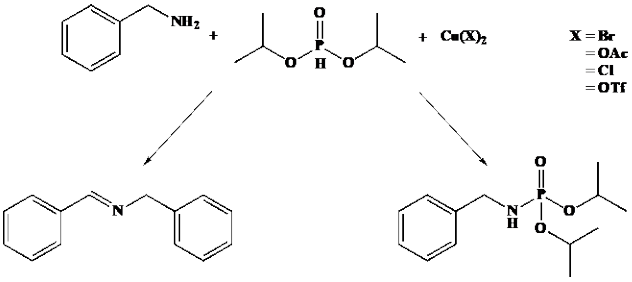

Scheme: Phosphoramidate and imine synthesis from benzylamine and diisopropylphosphite

23. Characterization of crosslinked materials from ε-polylysine and reducing sugars via the Maillard reaction

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ε-poly-L-lysine (ε-PL), a natural poly(amino acid), is produced from renewable resources such as sugars and amino acids by a kind of actinomycetes. The chemical structure of ε-PL is very similar to nylon 6 (Figure 1), which is a useful engineering plastic with excellent mechanical and thermal properties. Therefore, ε-PL is expected to be used as a polymer material with excellent mechanical/thermal properties. The biggest problem of ε-PL to apply it for a polymer material is its brittleness and low moldability into desired shape, which is due to high crystallinity and low molecular weight of ε-PL. To overcome this brittleness and low moldability of ε-PL, we introduced a crosslinked structure to ε-PL via the reaction between amino groups and reducing sugars (known as the Maillard reaction). Pure ε-PL became white and brittle fragments after the drying of aqueous solution (Figure 2, upper row), however, the mixture of ε-PL and reducing sugar (fructose) became transparent-orange, and flexible solid after the drying (Figure 2, lower row, named as ε-PL/sugar complex) despite the same drying condition. The ε-PL/sugar complex revealed a tensile strength of 27.9 MPa and Young's modulus of 741.6 MPa at the weight ratio of ε-PL:fructose = 60:40, which corresponds to those of high-density polyethylene (25 MPa and 760 MPa respectively). In addition, the ε-PL/sugar complex showed antimicrobial activity derived from the antimicrobialfeature of ε-PL. The good moldability, mechanical property, and antimicrobial activity are not possible in pure ε-PL, which will open new applications of biomass-derived ε-PL.

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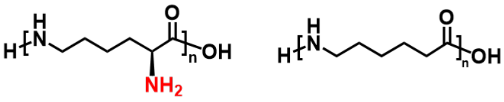

ε-poly-L-lysine (ε-PL)

Nylon 6

Figure 1: Chemical structure of ε-PL and nylon 6.

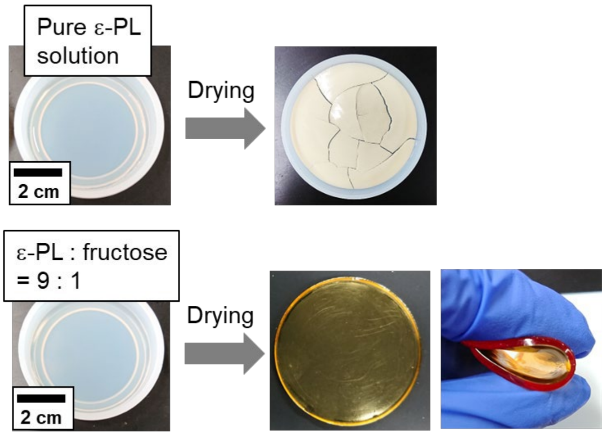

Figure 2: Apparence of pure ε-PL and ε-PL/fructose complex.

24. Interplay Between π-Conjugated Polymer Donors and Acceptors Determines Crystalline Order of Their Blends and Photovoltaic Performance

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Organic photovoltaics (OPVs) have been attracting much attention as a next-generation solar cell technology, because of the solution-processability, lightweight and flexibility, which allow us to install them in places where the conventional silicon photovoltaic cannot be installed. Although the power conversion efficiency (PCE) of OPVs has been low, the evolution of new organic semiconductors as photoactive materials has markedly improved the PCEs over 18%, approaching those of other photovoltaics[1].

Previously, our group has developed PTzBT (Figure 1a). With the donor (thiophene)–acceptor (thiazolothiazole) type backbone, PTzBT showed high crystalline structure in the thin film, leading to high charge carrier mobility[2)]. However, when PTzBT was blended with an n- type organic semiconductor to form a photoactive layer of the OPV cell, the crystallinity significantly varied by type of the n-type material, i.e., “fullerene” and “nonfullerene”, which affected the PCE of the cells. Therefore, achieving high crystallinity even in the blend film is crucial for achieving high PCEs. Here, we also prepared a derivative of PTzBT, named PTzBTE (Figure 1a), which possess alkyl and ester groups in the side chain, while PTzBT only possesses alkyl groups. Due to the intramolecular noncovalent interaction between oxygen of the ester group and sulfur of the thiazolothiazole ring, PTzBTE has a more rigid backbone, which is expected to improve the crystallinity of the polymer. These polymers were blended with several different n-type materials, including a fullerene derivative and non-fullerenes (Figure 1b), and their crystalline structures in the blend films and OPV performances were systematically investigated.

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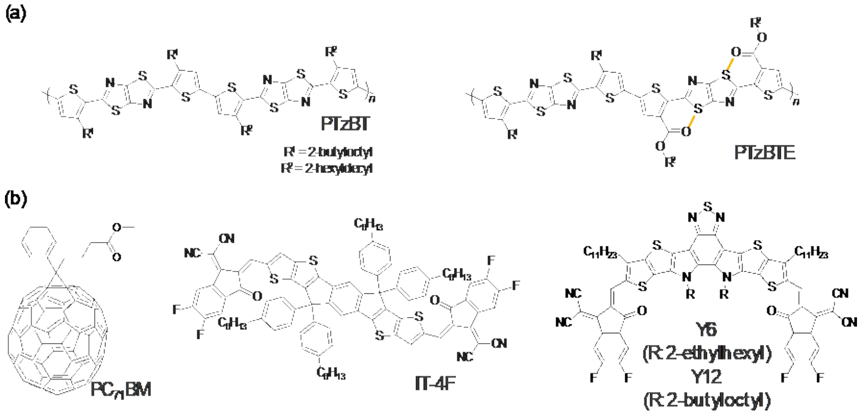

Figure1. Chemical structures of (a) thiophene and thiazolothiazole copolymer, PTzBT and PTzBTE, and (b) n-type organic semiconductors used in this study.

25. Alternating copolymerization of CO2 and cyclohexene oxide (CHO) to render polycarbonates under ambient conditions

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Application of carbon dioxide (CO_2) as a renewable raw material in production of pharmaceutical intermediates, materials, and other fine chemicals is attracting intensive interests. Among these application, an effective way to utilize CO_2 is the copolymerization of CO_2 and cyclohexene oxide (CHO) to render polycarbonate, which can be widely used in food packaging and adhesives, etc [1]. Currently, it is reported that several complexes can show good activity under 1 bar CO_2, but relatively high temperature is necessary for these catalysts [2]. Therefore, there are still great challenges to develop a copolymerization catalytic system with high activity and selectivity under ambient conditions. Our group reported the first example of an efficient rare earth metal RE-Zn heterometallic complex stabilized polydentate o-phenylenediamine-bridged tri(phenolate) ligand for copolymerization of CHO and CO_2 under mild condition (i.e., 25 °C, 7 bar CO_2) [3]. On basis of these studies, we herein developed the first RE-Mg heterometallic complexes that combines privileged ligand backbones, which are highly active and selective initiators for the copolymerization of CHO and CO_2 under ambient temperature and pressure (30 °C and 1 bar). In situ IR spectroscopy and ^{1}H NMR were employed to monitor the copolymerization. More importantly, cooperation between rare earth metal and magnesium centers proves crucial for the good performance.

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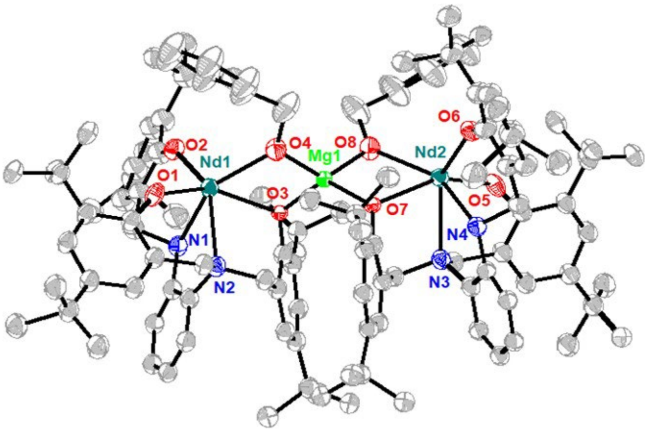

Figure: Solid state structure of Nd-Mg complex

26. Effect of sintering temperature on thermoelectric properties of BiCuSeO system

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During the past few decades, thermoelectric materials have attracted enough attention and are good candidates for green and flexible source of electricity. Thermoelectric generators are environmental friendly sources of energy. BiCuSeO has been studied comprehensively, especially after Zhao *et al.* [1], have reported intrinsically low thermal conductivity that varies from 0.45 to 0.9 $Wm^{-1}K^{-1}$ in a temperature range 300 - 923 K. Feng *et al* [2] prepared samples of BiCuSeO under three different temperatures and were sintered for different durations and found a peak ZT value of 0.62 at 873 K with ball milling duration of 16 h, whichincreased to 1.15 with the doping of Ca/Pb. In this report we have studied the influence of sintering temperature on the thermoelectric (TE) transport of BiCuSeO. The main aim is to optimize the processing conditions for higher TE transport. BiCuSeO samples were prepared at different sintering. A non-degenerate nature of conductivity is observed in all the samples at high temperatures. The Fermi level was positioned below the valence band maximum, thereby exhibiting a p-type degenerate transport in the entire range of temperature. It was witnessed that the variations of weighted mobility and power factor were found to have identical trends. The highest power factor was noticed at 554 K with a value of 129 $\mu Wm^{-1}K^{-2}$for the sample sintered at 673 K.

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27. Green and sustainable carbon dots for security printing applications

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Building a sustainable environment using renewable materials to minimise waste production have garnered prominent research attention. The present study highlights the reuse of carbon-rich biowastes as economical and green raw materials for the preparation of carbon dots with real life applicability. Pista shells composed of cellulose, hemicellulose, and lignin is effectively employed as a carbon rich source in the synthesis of carbon dots through carbonisation and green hydrothermal methods. The carbonaceous nanomaterial was column purified and the methanol fraction was chosen based on the fluorescence emission required for security application. The green and blue emitting carbon dots was further characterised using various analytical techniques to confirm the morphology, crystallinity, elemental composition, surface groups, and fluorescence lifetime. Further, the carbon dots were used as colourant material to formulate an environment friendly water-based security printing ink. The proofs obtained on UV-dull paper using screen printing exhibited good print properties. The yellow emission from the ink film upon shining with a 365 nm UV light sourcecan be used to check the originality of documents and for information storage.

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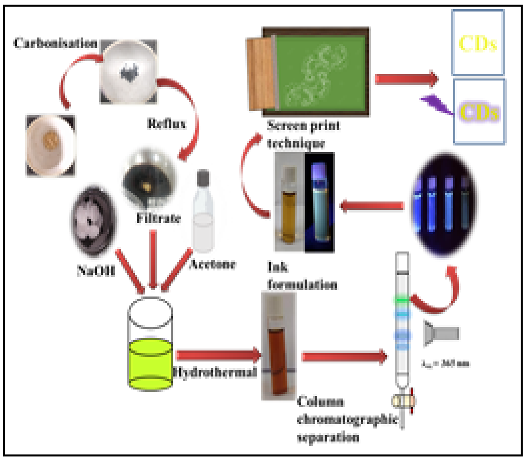

Figure: Screen printing using green carbon dots

28. Obtaining Important Nitrogen-Containing Compounds from the Valorisation of Chitin

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Chitin is the most abundant and accessible source of biologically fixed nitrogen and the second most abundant biopolymer on Earth. Chitin exists in the exoskeletons of arthropods and molluscs, and in the cell walls of certain fungi.[1] Approximately 6 to 8 million tonnes of crustacean shell waste is generated annually, which is used for low value applications or simply disposed of as part of municipal waste.[2] Most nitrogenous chemicals are currently derived from ammonia synthesised via the Haber-Bosch process. This nitrogen fixation process accounts for approximately 1.5% of global greenhouse gas emissions and produces the most CO_2 of any chemical manufacturing procedure.[3] Thus, the ability to convert chitin and its constituent monomer, N-acetylglucosamine, obtained from shell waste could reduce demand for the environmentally harmful Haber-Bosch process.

This poster presentation details investigations into the conversion of N-acetylglucosamine to an important nitrogen-containing platform chemical, 3-acetamido-5-acetylfuran (3A5AF), within different ionic liquid solvent systems.

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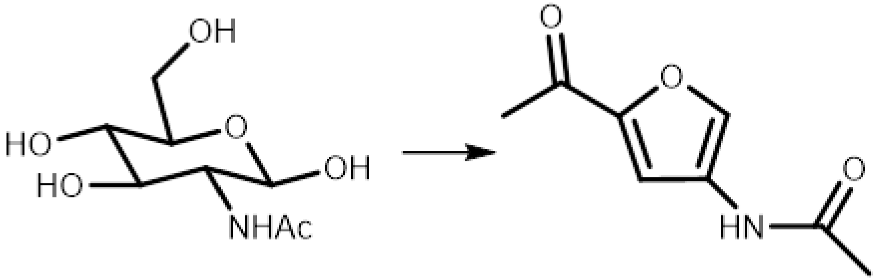

Figure: Structures of N-acetylglucosamine and 3-acetamido-5-acetylfuran

29. The Catalytic Conversion of Glucose to 5-Hydroxymethylfurfural in Nanostructured Ionic Liquids

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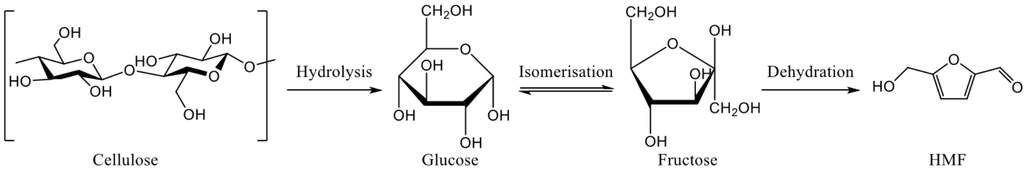
Lignocellulosic biomass is a feedstock of interest as an alternative to fossil fuels, as it can provide a source of biogenic chemicals, such as cellulose, outside of the human food chain. Lignocellulosic biomass sources represent an underused feedstock due to factors such as lignin content, the crystallinity of cellulose and its particle size, which limit the digestibility of hemicellulose and cellulose present.[1]

5-Hydroxymethylfufural (HMF) is an organic compound readily formed through the dehydration of sugars such as fructose, although it can also be obtained from cellulose. HMF is considered an important chemical intermediate due to its compatibility with many chemical processes and its potential availability from cellulosic sources (Scheme 1). A major challenge for HMF production has been the glucose isomerisation step and the solubility of cellulose and glucose to enable the reaction to occur. Ionic liquids (IL) represent some of themost effective solvent systems for these transformations although key structural factors suchas the influence of less strongly hydrogen bond accepting anions and the use of ILs with amphiphilic nanostructures is less well studied.[2]



Scheme 1: Multistep process for cellulose conversion to HMF.

This presentation will outline the effects that anion and alkyl chain length selection have on both the stability of HMF and efficiency of glucose conversion to HMF. The degradation of HMF and yields of HMF were analysed by HPLC. The stability of HMF within ILs was monitored over 24 h in the presence of both hydrochloric acid (HCl) and chromium (III) chloride ($CrCl_3$).

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30. Detection and Management of PFAS in Aotearoa

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Per- and polyfluoroalkyl substances (PFAS) are a class of thousands of man-made chemicals with a partially or fully fluorinated carbon chain. Developed in 1940s, these amphiphilic compounds, with a hydrophilic head and a hydrophobic tail, have unique properties to repel oil, water and grease and have excellent chemical, biological and thermalstability due to strong C-F bond (105.4 kcal/mol).[1] Thus, they have well-known uses in a variety of consumer and industrial products namely, waterproof clothing, non-stick cookware,food packaging, personal care products, electronics, stain-repellent carpets, lubricants, surface coatings and firefighting foams.[2] Due to their ubiquitous use and persistence, these highly mobile[3] *forever chemicals* have been detected across environmental media and evenin rain water,[4] indoor spaces,[5] food,[6] human blood[7] and breast milk[8]. Owing to their health and environmental concerns, and analytical improvements, there has been increased attention towards regulating, remediating, phasing-out, and substituting these Chemicals of High Concern (CoHC). Though PFAS are not manufactured in New Zealand, recent studies have found their occurrence in local common dolphins[9] and urban waters[10]. This presentation aims to highlight the occurrence of PFAS in Aotearoa, focusing on contaminated sites and results from PFAS in NZ household dust samples. Findings from adsorption studies conducted on newly synthesized sorbents for short and ultra-short chain PFAS removal from aqueous media will also be discussed. The current state of knowledge on emergence, distribution, remediation, and safe-by-design replacements to PFAS in Aotearoa will help raise awareness for this next global public health emergency.

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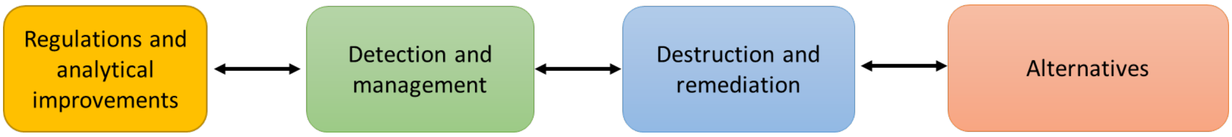

Figure: PFAS detection and management flow

31. Installing tunable functionality in polysulfides through inverse vulcanisation with silyl protected cross-linkers.

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The widespread use of petroleum-derived polymers has raised significant sustainability and environmental concerns, prompting the exploration of alternative resources.[1, 2] Surplus sulfur presents a promising solution, offering the potential to produce polysulfides with highly desirable properties. Inverse vulcanisation, a well-established polymerization technique that relies on the utilization of diene-containing cross-linkers, has demonstrated remarkable efficacy in stabilizing polysulfides with a unique set of characteristics, making them highly versatile and promising candidates for a wide array of applications.[3] This study focuses on producing functional polysulfides by leveraging a range of readily accessible organic molecules derived from natural resources, such as farnesol and eugenol, as cross-linkers. These molecules possess hydroxyl groups, making them suitable candidates for further functionalisation. However, a critical challenge arises with the reported loss of the hydroxyl (OH) group during the inverse vulcanisation reaction. To overcome this limitation, silylation reactions are employed to protect the OH group by forming silyl ether groups.[4] The incorporation of silylated organic molecules into the inverse vulcanisation reactions, changes the material's properties and the subsequent removal of the silyl protection group, will regenerate the reactive pendant OH groups on the surface. These groups can undergo post- polymerisation functionalisation reactions tuning the surface properties. These novel polysulfides offer a plethora of opportunities across diverse applications, such as being employed in coatings with appended specific functional groups. Additionally, they can serve as sorbents to recover heavy metals or sequester organic pollutants effectively.

The tunable properties of these polysulfides opens new possibilities for addressing various challenges across multiple industries.

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32. Efficient decomposition of ethylene-tetrafluoroethylene copolymer using subcritical water with alkaline reagent

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Fluoropolymers are high performance materials that allow high resistances to heat, chemicals, ignition, mechanical stresses, and UV-light irradiation. Among them, ethylene-tetrafluoroethylene copolymer (ETFE) is used as piping, wire insulation, protective films, fuel tubing and other purposes because it has combined characteristics of the high stability of fluoropolymers with the melt processability of common thermoplastic polyolefins. For the waste treatment, these polymers can be incinerated.1) However, this requires high temperatures to break the strong C–F bonds, and the released hydrogen fluoride gas can seriously damage the firebrick of an incinerator. Thus, in most cases, the wastes of these polymers are disposed of in landfills.[2]

If these polymers could be decomposed to F^- ions (i.e., undergo mineralization) by means of environmentally benign techniques, the established protocol for treatment of F^- ions could be used. Thus, Ca^{2+} is added to the system to form CaF_2, which is a raw material for hydrofluoric acid. We report herein an effective method for the mineralization of ETFE using subcritical water with an alkaline reagent.[3]

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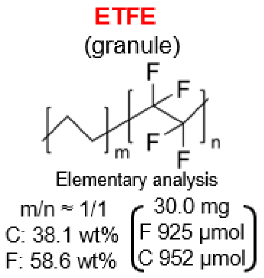

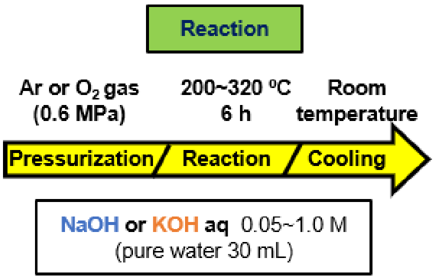

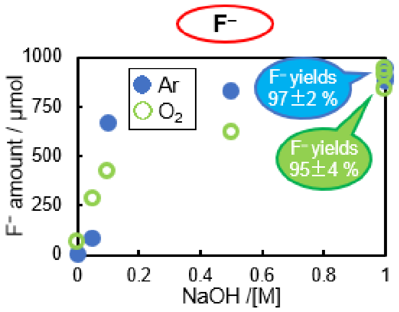

33. New Hydrogen-bonded liquid crystal supramolecular systems: Green Synthesis

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Novel H-bonded liquid crystals (HBLCs) are synthesized and examined for their mesomorphic behavior. All the compounds exhibit Smectic A mesophases, with one of thecompounds exhibiting LC properties below 25°C. Density functional theory (DFT) calculations revealed the formation of two hydrogen bonds between the substituted acids and the pyridine ring based on the orientation of the donor and the acceptor moieties.

Quantum chemical modelling studies on these molecules revealed the reduction in the HOMO-LUMO energy gap by approximately 0.3 eV for oxy-containing compounds, making them more chemically reactive by donating electrons (+I) into the aromatic cores. These materials provide a significant breakthrough in designing innovative LC materials. Hydrogen bonding is a significant soft covalent interaction prevalent in various systems. The building blocks of cells, the structures of proteins and DNA, the very crucial life- sustaining water molecules are all possessing the hydrogen bonds. The synthesis of liquid crystals involving hydrogen bonds is more sustainable as it involves non-corrosive chemicals and solvents in minimum quantities. The process is a simple single step condensation reaction with elimination of water molecule. The synthesized compounds are water soluble and thus contributes to the principles of green synthesis.

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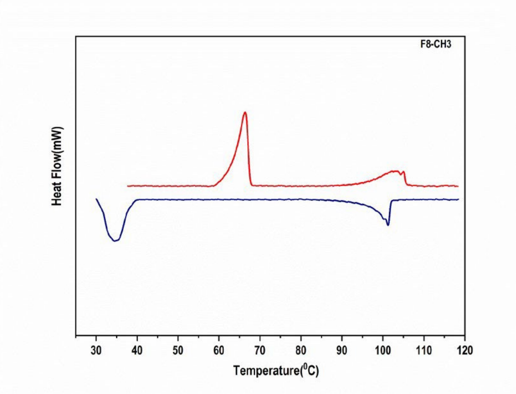

Figure 1:DSC thermogram of P8:CH_3

34. A potential green inhibitor for the corrosion mitigation of 6061 Aluminium alloy hybrid metal matrix composite in acid medium

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Carbohydrate compounds are recognized to be potent green corrosion inhibitors owing to their structural properties and eco-friendliness. The undertaken work shows the efficacy of glucosamine sulfate (GAS) as an eco-friendly green inhibitor to mitigate the deterioration of 6061 aluminum alloy reinforced with 2% SiC and 2% B_4C hybrid composite (AA-HMMC) material in 0.1 M hydrochloric acid (HCl) medium. Electrochemical measurements such as potentiodynamic polarization (PDP) and electrochemical impedance (EIS) were carried outto measure the corrosion rate in the absence and presence of GAS. Results were includedinto an acceptable adsorption isotherm model, and a suitable mechanism for the corrosion inhibition process was provided. To comprehend the method of adsorption, the Freundlich isotherm model was applied. The techniques of SEM, AFM, and XRD were used to verify the adsorption of the investigated inhibitor.

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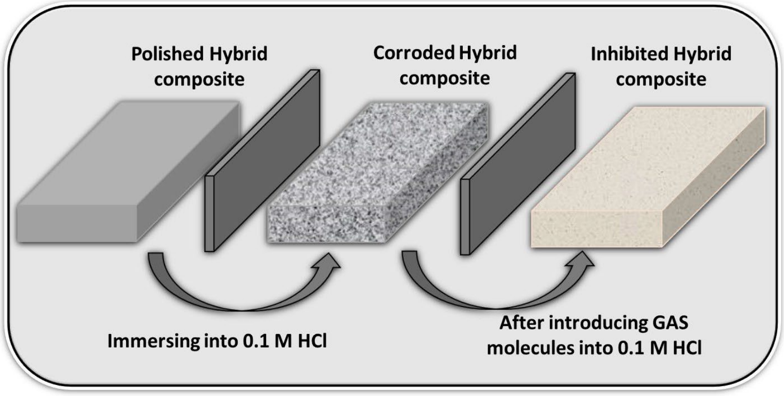

Figure: Graphical representing the corrosion process

35. MODIFICATION OF HEMPSEED PROTEIN ISOLATE'S PHYSICOCHEMICAL PROPERTIES USING HIGH-PRESSURE HOMOGENIZATION AND HIGH-INTENSITY ULTRASOUND

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Compared to traditional animal-based proteins, plant protein is attracting more attention due to its environmental sustainability. Hempseed protein isolate (HPI), derived from hempseed, shows great potential for development as a food protein, as it is nutritious, easily digestible, and low-allergenic[1]. However, the HPI has poor solubility, which limits its application in the food industry[2]. High-pressure homogenization (HPH) and high-intensity ultrasound (HIU), asenvironmentally friendly technologies, have been found to enhance the solubility of the protein[3]. However, the effect of a single technology is limited and cannot satisfy the need for functionality. Therefore, in this study, we aimed to combine the HPH with HIU (HU) to modify the HPI and studied its physicochemical properties. The results showed that compared with the single-HPH and single-HIU treatment, HU treatment could maximally improve the solubility of HPI, and reduce the particle size to the minimum value. In addition, after HU treatment, the content of α-helix was decreased, and the content of the random coil was increased, it indicated that the structure of HPI was unfolded, and the active groups were exposed to the surface of HPI. It was also confirmed by the decrease in the total sulfhydryl content and the increase in fluorescence intensity and surface hydrophobicity. These changes facilitated the water-protein and oil-protein interactions. As a result, the foaming and emulsifying properties of HPI were improved. The results of this study have proven that HU as green processing technology is useful to expand the application of HPI in the future food industry.

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36. Steel Decontamination using a Regenerative Deep Eutectic Solvent-Ion Exchange System for Radionuclide and Heavy Metal Removal

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Nuclear waste presents a significant challenge due to the generation of radioactive isotopes (RIs) and potential contamination risks. Moreover, there has been on-going concern with surface decontamination of Stainless Steel (SS), where it has been observed that the formation of a radioactive contaminant layer consisting of RIs and heavy metals can be generated.[1] Contamination through decommissioning processes is a major concern.
Therefore, the development of alternative green, cost-effective, and efficient separation tools is essential to aid waste volume reduction and the production of greener waste forms, in turn crucial for nuclear energy to provide clean energy and meet increasing electricity demand while minimizing its harmful waste generated.[2] Furthermore, non-environmentally friendly chemical reagents used for decontamination compound the pressure of rapidly filling interim storage facilities for nuclear waste.[3]

In this work we have developed an efficient, cost-effective and green technology for the decontamination of SS surfaces, and the separation and recovery of RIs. The complete removal of the metal oxide contaminant layer on SS304 using choline chloride – *p*-toluenesulfonic acid (ChCl:PtsA) DES at room temperature was successful, leaving contamination-free SS.

The addition of IX media into hydrated DES can result in the effective separation of contaminants now present in the DES. This system has the potential to overcome challenges faced in nuclear waste management. Generating an understanding of how DESs interact with the selected RIs and how they also interact with IX media will ultimately allow for a proof-of-concept and the design of DES-IX systems for other environmental and waste remediation processes.

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37. Ionic liquid as green corrosion inhibitor for 6061Al-10vol% SiC(p) composite in HCl

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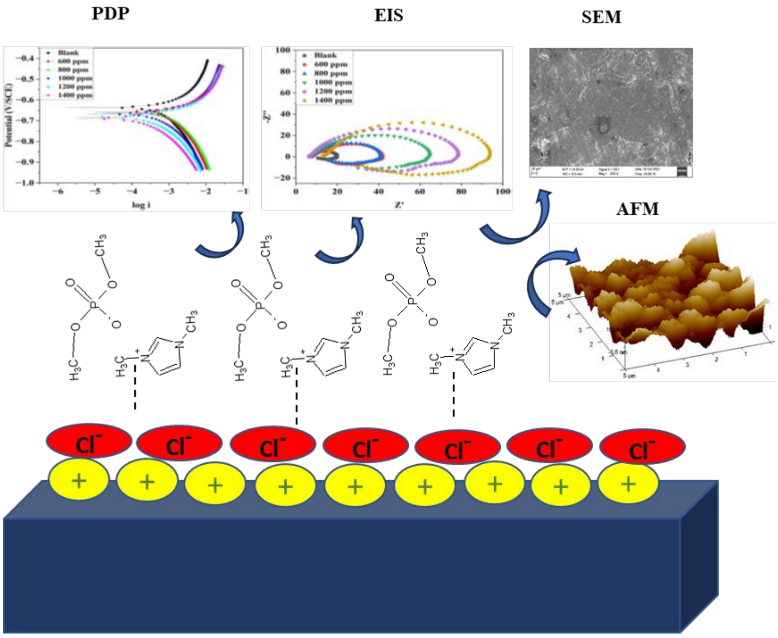
The inhibition efficiency of an eco-friendly ionic liquid 1,3 dimethyl imidazolium dimethyl phosphate (DIDP) on the corrosion behaviour of 6061Al-10vol% $SiC_{(P)}$ composite in 0.25 M HCl solution has been investigated in the temperature range 303 - 323 K using electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization (PDP) technique. Conditions were optimized to achieve maximum inhibition efficiency by varying inhibitor concentration and temperature. Kinetic and thermodynamic parameters were calculated using the Arrhenius rate law and transition state equations. The results indicate that possible green inhibitor DIDP is physisorbed obeying Freundlich adsorption isotherm. The inhibitor efficiency increases with increase in inhibitor concentration and with increase in temperature the efficiency decreases for a given inhibitor concentration. The maximum efficiency was about 80% for 1400 ppm of DIDP at 303 K. Surface morphology was studied both in presence and absence of inhibitor by techniques such as SEM, AFM, and EDAX.



38. Vapor-liquid equilibria in the 1-methylpyrrolidine + 1-butylimidazole binary system: Experimental measurements and theoretical modelling

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In this study, we performed a comprehensive examination of the 1-methylpyrrolidine (nMPi)+ 1-butylimidazole (nBI) binary system to provide a useful foundation for process simulation. The potential industrial applications[1,2] and hazardous nature of nMPi and nBI chemicals are highlighted, emphasizing their impact on the environment.[3,4] The study focuses on determining the vapor-liquid equilibrium (VLE) data and appropriate models for kinetic and thermodynamic research, mass balance calculations, and process modeling. Using obtained VLE data, the binary interaction parameters (BIP) were regressed by maximum likelihood method for non-random two-liquid (NRTL)[5] activity coefficient model with Hayden-O'Connell (HOC)[6] equation of state, as well, BIP were regressed for: universal quasichemical (UNIQUAC),[7] Van Laar,[8] and Wilson[9] activity coefficient models. Thermodynamic consistency was confirmed by applying the Redlich−Kister area test. Despite their significantindustrial importance, limited studies have been conducted on the thermodynamic, physical, and chemical properties of pure nMPi and nBI chemicals, as well as their binary system.

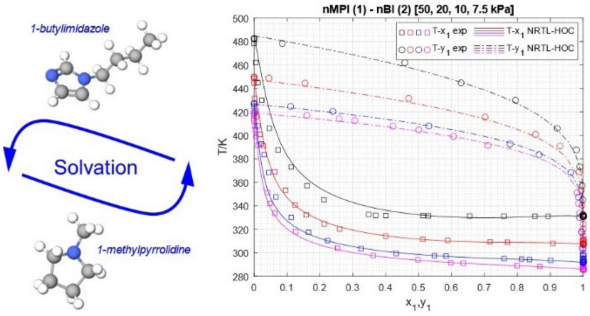

Figure 1: Graphical Abstract

This study aims to fulfill the existing knowledge gaps, ultimately proving useful information for future process simulations. Therefore, the vapor pressure of nBI was determined by direct measurement of the equilibrium temperature at different pressures. The Antoine equation parameters were regressed for nMPi and nBI. In addition, dipole moment (μ) values were evaluated by quantum chemical calculations using the Hartree–Fock (HF) method through GAMESS package. The density, the sound velocity, the refractive index, and the normal boiling points were also measured for binary mixtures and pure components.

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39. Green liquid catalysts for Diels-Alder reactions

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Fluorinated compounds such as 1,1,1,3,3,3-hexafluoroisopropanol (HFIP) and trifluoracetic acid (TFA) are commonly used as catalysts and solvents for many reactions such as the Diels-Alder reactions shown in Figure 1.[1,2]

In this work a class of liquids has been identified as a potential green catalyst alternative for use in these reactions.

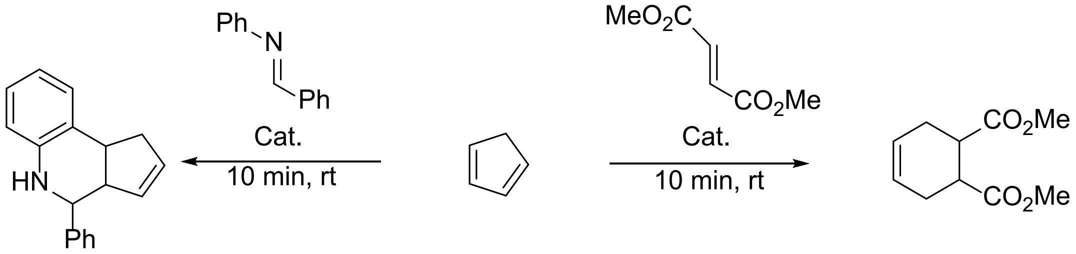

Figure 1: Model Diels-Alder reactions.

This presentation will elucidate the rate accelerating effect observed with this class of liquid catalyst and investigate the scope for use of these as green catalysts beyond the Diels-Alder reaction.

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40. Methylation with dimethyl carbonate/dimethyl sulfide mixtures: an integrated process without addition of acid/base and formation of residual salts

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Dimethyl carbonate (DMC) has recently been used as a green solvent and a methylating agent for a wide variety of substrates, such as phenols.[1,2] It is a promising green reagent for replacing conventional methylating agents, such as methyl halides and dimethyl sulphate, which are environmentally unfriendly. By using DMC in methylations, the production of inorganic waste salt can also be avoided resulting in enhanced atom economy. In this study, a novel catalyst dimethyl sulfide is used to perform DMC methylations and the products are purified simply by evaporation. Besides *O*-methylation of phenols reported previously, *O*-methylation of benzoic acids and *C*-methylation of phenylacetonitriles (eg. 4-nitrobenzoic acid, 4-fluorophenylacetonitrile) were also methylated using the optimized conditions (220°C, 4-6 hours) with excellent yields. GC-MS and ^{1}H-NMR were used to identify and quantify both major and minor products. >90% yield was obtained for almost all the selected substrates. The mechanism of the methylation reaction has also been elucidated. Dimethyl sulfide and DMC reacts at high temperature to form a very reactive ionic species, $[Me_3S]^+[OCO_2Me]^-$. The $[Me_3S]^+$ cation acts as an alkylating agent in the methylation reaction. This has been elucidated by observing phenyl butyl ether/phenyl octyl ether and but-1-ene/oct-1-ene when reacting DMC with dibutyl sulfide and di-*n*-octyl sulfide.[3]

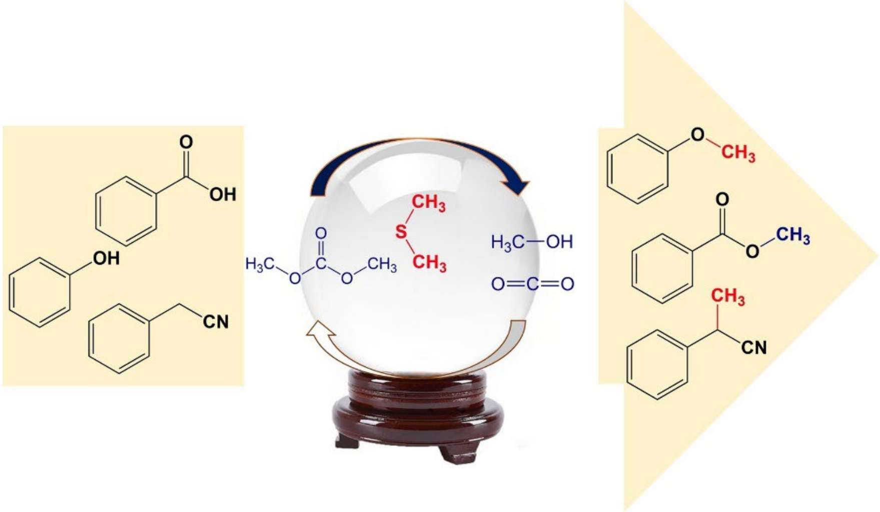

Figure: Methylation of phenols, phenolic acids and phenylacetonitriles using DMC and dimethyl sulfide with MeOH and CO_2 by-products.

41. Potassium catalyzed pyrolysis and low temperature CO2/O2 gasification of woody biomass in a two-stage reactor

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In this work, an advanced and efficient strategy for total conversion of lignocellulosic biomass into syngas by CO_2 gasification has been proposed. The novel type of gasification process based on the proposed strategy consists of pyrolysis of woody biomass at 550 °C, followed by CO_2/O_2 reforming/gasification of resulting volatiles/char around 730 °C. Potassium (K) is loaded over the feedstock biomass for enabling low temperature reforming/gasification. The endothermic reforming/gasification is also utilized for chemical quenching of hot syngas. By these features, the process has a potential to yield syngas with an exceptional cold gas efficiency (i.e., chemical energy recovery) of 95% or even higher, based on the lower heating value (LHV). This work aimed to prove the concept of this two-stage gasification using a woody biomass as feedstock by experimentally demonstrating near-complete conversion of carbon in biomass to syngas with extremely low concentration of tar in it. In the experiment, the effects of key operating variables, such as CO_2/C ratio, O_2/C ratio, K loading amount and gasification temperature, on the process performance are systematically investigated. As a result, the gasification of 1 mol K-loaded biomass (1 mol-K/kg-dry-biomass) realized steady-state carbon conversion around or more than 100% together with tar concentration in the dry syngas well below 10 mg/Nm^3 at $CO_2/C > 0.40$ and $O_2/C > 0.28$.

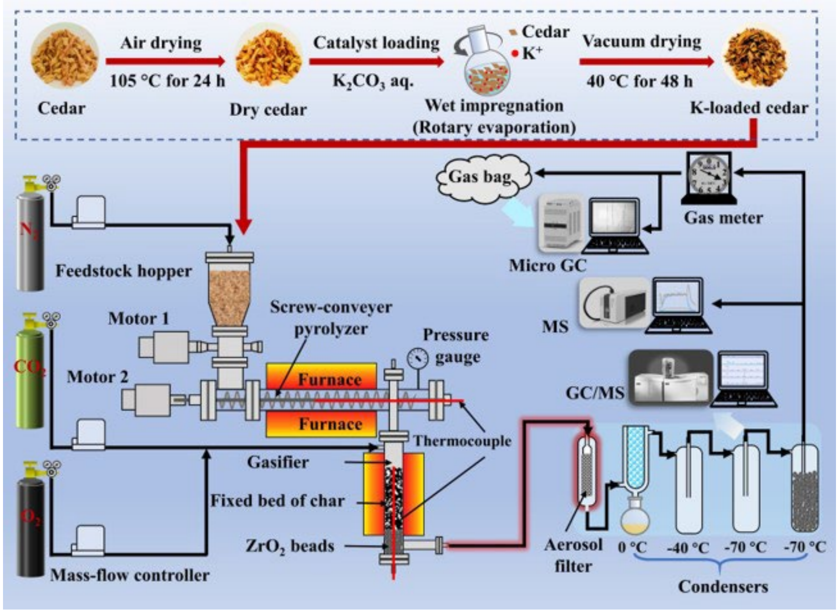

Figure: Schematic diagram of K-catalyzed pyrolysis and CO_2/O_2 gasification of woody biomass in a two-stage reactor.

42. Alkaline hydrothermal reduction of CO2 with bio-oil model compound as reductant and carbon source to produce formic acid

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Carbon recycling technologies, as part of CCU technologies, have attracted great attention due to environmental concerns. Formic acid (FA) is an attractive CO_2-derived product as a hydrogen storage carrier and feedstock for a variety of chemicals. FA production with CO_2 generally considers its hydrogenation, which requires hydrogen. An emerging method is the alkaline hydrothermal reduction of CO_2. CO_2 is dissolved in NaOH aqueous solution, producing $NaHCO_3$, and then heated in the presence of a reductant under hydrothermal conditions to produce FA. Hydrogen source in this case is water and the reductant. Interestingly, the carbon source for FA is not only CO_2, but also the compound is used as the reductant. Past studies employed alcohols and glucose as the reductant, but their production from biomass poses a problem of cost. In this work, bio-oil, easily accessible from biomass, is considered as an alternative reductant. The major part of compounds contained in the oil have a potential to serve as the reductant and FA source. Prior to the investigation of bio-oil, this work studied performance of levoglucosan (LGA) as the reduactant. LGA is generated from cellulose during the biomass pyrolysis and one of main components in the oil. The analysis of its reaction during the hydrothermal treatment (HT) with $NaHCO_3$ aqueous solution provides important insight into the bio-oil reaction system. The experiment revealed its effect for yielding more FA, compared to the reaction with glucose as the reductant, and mechanisms leading to the FA formation.

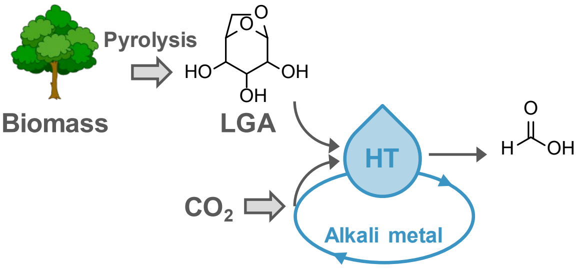

Figure: Alkaline hydrothermal conversion of CO_2 and LGA to FA

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