ScotCHEM

Polymer & Soft Materials Conference II

THURSDAY, 4 MAY 2023

T100 LECTURE THEATRE,
JOSEPH BLACK BUILDING,
UNIVERSITY OF EDINBURGH

BRINGING TOGETHER RESEARCHERS FROM ACROSS SCOTLAND WORKING IN POLYMER CHEMISTRY AND SOFT MATERIALS AND SHOWCASING RECENT ADVANCES IN THE FIELD

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ScotCHEM Polymer & Soft Materials Conference II

T100 LECTURE THEATRE, JOSEPH BLACK BUILDING, UNIVERSITY OF EDINBURGH

THURSDAY, 4 MAY 2023

AGENDA

09:30 – 10:00	Arrival, Registrations, Coffee and Placing Posters
10:00 – 10:05	Welcome: Prof Bill MacDonald, ScotCHEM
Session 1	
10:05 – 10:45	Dr Amit Kumar 'Homogeneous (De)hydrogenative Catalysis for A Circular Economy'
10:45 – 11:25	Dr Ruaraidh McIntosh 'Balancing Sustainability with Activity in Polymerisation Catalysis'
11:25 – 12:05	Dr Paul Hunt 'Practicality of Making Sustainable Polymers'
12:05 – 13:30	Lunch and Poster Session
Session 2	
13:30 – 14:10	Dr Emily Draper 'Using Supramolecular Assembly for Flexible Organic Materials'
14:10 – 14:50	Prof Mike Ingleson 'Electrophilic Borylation as a Route to Generate Deep LUMO / Near IR-Emitting Small Molecules and Polymers'
14:50 – 15:20	Coffee Break and Posters
Session 3	
15:20 – 16:00	Dr Ketan Pancholi 'Magnetic Polymer Nanocomposites Incorporating Metal-Organic Frameworks: Tailored Synthesis for Targeted Applications'
16:00 – 16:40	Dr Ross Minty 'The Role of Residual Stress at the Fibre-Matrix Interface in Composite Materials'
16:40 – 16:50	Closing Remarks and Poster Prizes
16:50 – 18:00	Drinks Reception

SESSION 1 PLENARY TALKS

ScotCHEM Polymer & Soft Materials Conference II

Speaker 1: Dr Amit Kumar, University of St Andrews

Homogeneous (De)hydrogenative Catalysis for A Circular Economy

The development of sustainable methods for the closed-loop production and recycling of plastics especially from renewable feedstock is an important challenge of current times. Reactions based on catalytic (de)hydrogenation are atom-economic and sustainable routes for organic transformations. Using the following two examples, this lecture will discuss the application of homogeneous (de)hydrogenative catalysis for the synthesis and degradation of plastics to enable a circular economy:
(a) synthesis of polyamides/nylons from the ruthenium catalysed dehydrogenative coupling of diamines and diols and its reverse reaction i.e. hydrogenative depolymerisation of nylons (Figure 1A)[1], and (b) the synthesis of polyureas from the ruthenium or manganese catalysed dehydrogenative coupling of diamines and methanol[2], and its reverse reaction, i.e. hydrogenative depolymerisation of polyureas (Figure 1B).[3] Preliminary results on the application of polyureas made using this method to advance Li-O2 battery will also be discussed.[4] Furthermore, the development of a new catalytic method for the synthesis of polyethyleneimines from the dehydrogenative coupling of safer and renewable feedstock (ethylene glycol and ethylene diamine) will also be discussed.

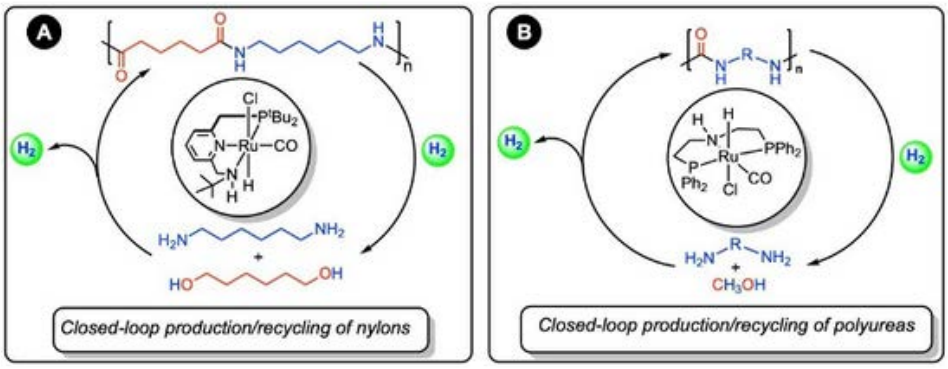

Figure 1. Synthesis and degradation of nylons (A), and polyureas (B) using (de)hydrogenative coupling of diamines and alcohols catalysed by ruthenium pincer complexes.

References:

1. A. Kumar, N. von-Wolff, M. Rauch, Y. Q-Zou, G. Shmul, G. Leitus, L. Avram, D. Milstein, J. Am. Chem. Soc., 2020, 142,14267-14275.
2. (a) A. Kumar, D. Armstrong, G. Peters, M. Nagala, S. Shirran Chem.Commun. 2021, 57, 6153-6156; (a)A. Owen, A. Preiss, A. McLuskie, C. Gao, G. Peters, M. Buehl, A. Kumar, ACS Catalysis, 2022, 12, 6923.
3. A. Kumar, J. Luk, Eur. J. Org. Chem.,2021, 32, 4546-4550.
4. R. Haas, L. J. Kaufer, C. Gao, A. McLuskie, G. Peters, A. Kumar, D. Schröder, 2022, ChemRxiv, DOI: 10.26434/chemrxiv-2022-ll9p1.

SESSION 1 PLENARY TALKS

ScotCHEM Polymer & Soft Materials Conference II

Speaker 2: Dr Ruaraidh McIntosh, Heriot-Watt University

Balancing Sustainability with Activity in Polymerisation Catalysis

As we transition away from an oil-based economy, one of the challenges faced is utilising the remaining resources in a sustainable way. Catalysis will play a key role in this but it is typically reliant on a small number of scarce elements and the ligand supports can involve complicated synthetic routes. Catalytic processes which utilise highly abundant metals, simple ligands and yield (relatively) stable complexes with high activity would be a highly desirable goal. One obvious target is to utilise renewable resources to replace the current oil-derived polymers. The catalytic ring-opening polymerisation of cyclic esters to form degradable polymers is an intensely studied area of chemistry; however, the most highly active initiators are typically very sensitive to degradation upon contact with trace moisture. Therefore, the development of more robust catalysts which do not require repeated purification of the monomers and dry solvents would be desirable. Unfortunately, the stabilisation of the catalyst typically comes at cost of activity, therefore innovative approaches to retain high activity while achieving a degree of stability are required. One potential method to stabilise the catalysts is the utilisation of supramolecular interactions, which can inhibit further degradation when the catalyst is not in use.

Speaker 3: Dr Paul Hunt, Croda Europe Limited

Practicality of Making Sustainable Polymers

Sustainability has become a major theme within the chemical industry (and beyond!), ranging from the raw materials we use right through to the manufacturing process. This presentation is to share what sustainability means to Croda, what we mean by a sustainable polymer, and how we take an idea from concept to commercial scale.

SESSION 2 PLENARY TALKS

ScotCHEM Polymer & Soft Materials Conference II

Speaker 1: Dr Emily Draper, University of Glasgow

Using Supramolecular Assembly for Flexible Organic Materials

Small organic molecules have the unique potential to being chemically altered so that they may be used for many different applications, such as small wearable devices, catalysis, displays, lighting, etc. On top of this, they also can be assembled and processed to further tailor their properties. However, where organics often fall down in these applications is in the lifetime, cycling and robustness compared to that of their metal counterparts. However, with rapidly depleting metal resources and reports of organic devices now outperforming metal ones, organics are now being taken more seriously for these applications. Our work looks at the self-assembly and processing of small molecules functionalised with amino acids in water for different organic electronic applications. We are aiming to address the issues that can let organic devices down when compared to metal-based electronics. The Draper group has focused on perylene bisimides, and naphthalene diimides and using them in applications such as mechanoresponsive, photoresponsive and electrochromic devices. We have found that the aggregation of the molecules in water has a huge influence on the behaviour of the final materials, such as conductivity, colour, longevity and lifetime of the samples, and so in turn, what they can be used for. By trying to understand the self-assembly of the molecules, and how this can be influenced by chemical structure, pH, and additives, we believe we can improve the properties of small organic materials so that they are comparable to that of their metal counterparts. We use techniques such as small angle neutron scattering, rheology, electrochemistry, UV-vis absorption spectroscopy and NMR combined with computational modelling in order to try and understand how these molecules self-assemble to form aggregates. This understanding gives us the unique opportunity to tailor our materials for flexible applications, just by changing the assembly conditions.

SESSION 2 PLENARY TALKS

Speaker 2: Prof Michael Ingleson, University of Edinburgh

Electrophilic Borylation as a Route to Generate Deep LUMO / Near IR-Emitting Small Molecules and Polymers

In this presentation, the use of BX3 (X = Cl or Br) as a simple route to functionalise conjugated materials (both small molecules and polymers) will be discussed. This enables the incorporation of 3 or 4- coordinate boron centres into organic materials. Boron incorporation significantly impacts key properties, particularly the LUMO energy which is often stabilised significantly post borylation. Several case studies will be presented, including the conversion of polymers such as poly(9,9-dioctylfluorene-alt-benzothiadiazole into efficient near-IR emitters on electrophilic C-H borylation.

SESSION 3 PLENARY TALKS

ScotCHEM Polymer & Soft Materials Conference II

Speaker 1: Dr Ketan Pancholi, Robert Gordon University

Magnetic Polymer Nanocomposites Incorporating Metal-Organic Frameworks: Tailored Synthesis for Targeted Applications

The design and synthesis of magnetic microporous porphyrazines have garnered significant interest due to their ability to improve catalytic efficiency and reduce excessive runaway of the catalyst. One promising approach to enhancing the rate of reaction is to attach a metal-organic framework (MOF) to a microporous membrane reactor, which can increase surface area and prevent water-soluble porphyrazines from escaping into the reactant flow.

In this study, we developed magnetic microporous porphyrazine-based MOF polymer nanocomposites and immobilized them onto an inert polymer membrane for catalytic reactions. Inert polymer membranes are ideal for use as reactors, as they can separate gases and provide a benign environment for the reaction. However, attaching MOF to such membranes presents a significant challenge.

Our initial results demonstrated that the prepared composite was able to catalyze the reaction via diffusion through pores, thereby increasing efficiency by 20%. MOF were grown on the surface of the composite, and their metal sites facilitated catalysis. This method holds promise for potential use in biomedical applications.

SESSION 3 PLENARY TALKS

Speaker 2: Dr Ross Minty, University of Strathclyde

The Role of Residual Stress at the Fibre-Matrix Interface in Composite Materials

It is well known that the fibre-matrix interface plays a key role in defining the mechanical properties of fibre composite materials. The ability to efficiently transfer stress between the matrix and the fibres is critical in ensuring the required performance level needed for advanced composite materials. Stress transfer across the fibre-matrix interface is often reduced to a discussion of 'adhesion'. Past discussions of thermosetting matrices have typically focussed on the chemistry of the matrix system, specifically the task of maximising the level of chemical bonding between the fibre and the matrix to produce the strongest interface. However, many authors have also commented on the potential for residual radial compressive stresses formed at the interface to be a significant contributor to the strength of the interface. There is still a significant weight of opinion that holds that even if these residual stresses at the interface can contribute to the stress transfer capability, then chemistry and chemical reactions must play an active role in defining their magnitude.

This presentation will explore the research led by Dr Minty, furthering our understanding of how chemistry and residual stresses formed at the interface could be interrelated to influence the stress transfer capability of the interface.

POSTER PRSENTATIONS

ScotCHEM Polymer & Soft Materials Conference II

Poster 1
Presenter: Maisarah Abdul Rahman, University of Edinburgh
Title: A Game of Tug-of-War: Balancing Enhanced Activity and Control in Multimetallic Complexes for Block Copolymer Synthesis

Poster 2
Presenter: Claire N. Brodie, University of St Andrews
Title: The Manganese CatalysedDehydrative Coupling of Amines and Alcohols to Polyethyleneimine

Poster 3
Presenter: Connor MacDonald, University of Glasgow
Title: Prediction and Testing of Self-Assembled Aggregates for Flexible Devices

Poster 4
Presenter: Timothy J. D. McCabe, University of Strathclyde
Title: Computer-vision Assisted Colorimetric Analysisof the UV-promoted Degradation of Polyurethane Foams

Poster 5
Presenter: Meltem Haktaniyan, University of Edinburgh
Title: Antibacterial Homopolymers bearing Quaternary Ammonium Groups

Poster 6
Presenter: Hamish William Alan Swanson, University of Strathclyde
Title: Minimal Peptoid Assembly: A Computational Rationale

Poster 7
Presenter: Isabel He, University of Edinburgh
Title: Synthesis and Analysis of Boron/Nitrogen Analogues of Spirobifluorene-Based Porous Polymers

Poster 8
Presenter: Chunchun Ye, University of Edinburgh
Title: Ion-SievingPolymer Membranes for Flow BatteryEnergy Storage

Poster 9
Presenter: Joseph W. Walker, Heriot-Watt University
Title: Rare Earth NHC Complexes For Biopolymer Synthesis

POSTER PRSENTATIONS

ScotCHEM Polymer & Soft Materials Conference II

Poster 10
Presenter: Anna Lykkeberg, University of Edinburgh
Title: Bifunctional Potassium Salts: Accessing Polyester-Poly(vinyl acetate) Block Copolymers through ROCOP and RAFT

Poster 11
Presenter: Nicholas Murray, University of Glasgow
Title: Naphthalene Diimide-Based Chromic Films

Poster 12
Presenter: Angharad Wood, University of Strathclyde
Title: Optimisation of Alginates for Packaging Applications

Poster 13
Presenter: Dominic Wadkin-Snaith, University of Strathclyde
Title: Using Simulation to Construct DesignRules for Compostable Plastic Packaging

Poster 14
Presenter: Nisha Middleton, University of Strathclyde
Title: Molecular Dynamics Simulations of Sustainable, Semi-crystalline Polymers

Poster 15
Presenter: Ian J. Bennett-Wright, Universities of Edinburgh and Glasgow
Title: The Properties and Tunable Nature of Electrochemically-Grown Dipeptide-Based Hydrogels at Single Microelectrodes

Poster 16
Presenter: Samuel B. H. Patterson, Heriot-Watt University
Title: Development of Photoactive Carriers for the Stimulated Release of Agrochemicals

Poster 17
Presenter: Emma Edwards, University of Strathclyde
Title: Investigating the Effect of Succinylated Content on the Properties of Gelatin Hydrogels

Poster 18
Presenter: Tom Swift, University of Bradford
Title: Polymer Additives as Modulators of Skin Contact Biomaterials

Poster 19
Presenter: Meng Wang, University of Manchester
Title: Polymeric Frustrated Radical Pairs for Networks Synthesis and Photocatalysis