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

Thank you to our sponsors:

Thank you to our Exhibitors:

With grateful thanks to the conference organising committee: Dr Utku Yolsal, Dr Jennifer Garden, Dr Raju Chambenahalli, Jack Hughes, Maisarah Abdul Rahman, Anna Lykkeberg, Peter Shaw and Eva Spanachi
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
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:
Speaker 2: Dr Ruairaidh 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.
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.
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.
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 porphyazine-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.
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 PRESENTATIONS**

**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 Catalysed Dehydrative 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 Analysis of 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-Sieving Polymer Membranes for Flow Battery Energy Storage

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

**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 Design Rules 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