Recent Appointees Workshop
ECR Flash Presentations
Early Career Researchers
Dr Graeme Barker
Heriot Watt University
Graeme Barker: Methodology

\[ \text{N=N} \quad \text{N=N} \]

1. 3.0 eq. \( \text{^nBuLi} \)
   0 °C, THF, 3 h

2. 4.0 eq. \( \text{E}^+ \)

- 18 Examples
- \( \leq 91\% \) yield
- Important pharmaceutical motif

requires \( \sim -30 \, ^\circ \text{C} \) in batch

\[ \text{N=N} \quad \text{N=N} \]

usable at rt in flow

- 33 Examples
- \( \leq 100\% \) yield
- Also important pharmaceutical motif

cAMP binds at interface to stabilise active EPAC state

E. Parnell et al., Trends Pharmacol. Sci., 2015, 36, 203
Dr Nicholle Bell
University of Edinburgh
Dr Damiano Bonaccorso
University of St Andrews
Dr James Cumby
University of Edinburgh
Dr Robert Edkins
University of Strathclyde
Robert Edkins
University of Strathclyde

Understanding optical properties of molecules

Design of new molecules for optical applications

Fundamental photophysics

Optoelectronics

Sensing

Bioimaging

Two-photon, FLIM & STED

Photodynamic therapy

@R_M_Edkins
Robert Edkins
University of Strathclyde

Understanding optical properties of molecules

Design of new molecules for optical applications

Triarylboranes
- Strong π-acceptors
- Reduction to radicals

Phthalocyanines
- Singlet oxygen photosensitization

Inorganic Heterocycles
- Phospholes
- Boroles

Organic chromophores
- Pyrene derivatives
- Photochromic imidazoles

Acknowledgements
- The group + funding

Phospholes

Boroles

@R_M_Edkins
Dr Jennifer Garden
University of Edinburgh
Dr Mairi Haddow
Heriot Watt University
Automated modelling of disordered molecules in crystal structures

Dr Mairi Haddow

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Dr Gordon Hedley
University of Glasgow
Organic Semiconductors
- Novel carbon based materials that conduct electricity & absorb & emit light
- OLEDs now widely used as displays in phones & TVs
- Can also be used in solar cells

What Can We Learn?
- What limits device efficiency
- Fundamental photophysical properties of molecules
- Pathways to novel materials
Dr Claire Hobday
University of Edinburgh
Dr Aruna Ivaturi
University of Strathclyde
Dr Amanda Jarvis
University of Edinburgh
**Motivation - Sustainable Catalysis:**

- Atom economic
- Sustainable
- Selective functionalisation

**Tool - Artificial metalloenzymes:**

Combining small molecule transition metal catalysts with protein scaffolds.

**Benefits of ArMs:**

- Control of substrate orientation – chemo, regio and enantioselective reactions
- Evolvable – high throughput optimisation
- Possibility of catalysts recovery – biphasic system
- Potential for in vivo catalysis, new cascades etc

Cellular factories?

www.amandajarvis.co.uk
By combining N- and P-cofactors with cysteines, we have access to a large

Artificial metalloenzyme design

\[
\text{SCP-2L} + \text{ACP} + \text{Fe, Ru, Pd, Cu, Rh, Mn} = \text{Novel enzymes for oxidation, hydroformylation, cross-coupling reactions etc}
\]

Can ArMs provide solutions where small molecules catalysts have not?

Evolvable ArMs using genetic code expansion to include Bipyridyalanine

\[
\text{N} = 15:85 \text{ e.r.}
\]

Opportunities for collaboration

- Biological/Homogeneous catalysis cascades
- High throughput method development
- Catalyst Characterisation
- New protein scaffolds

Other applications for these constructs?
Dr Craig Johnston
University of St Andrews
The Importance of Chirality

Dr Craig P. Johnston, Royal Society University Research Fellow, University of St Andrews

enantiomers

enantiomers

(S)-Naproxen
treatment for arthritis

(R)-Naproxen
toxic to the liver
Sustainable Enantioselective Catalysis

- Novel chiral building blocks for organic synthesis
- Late-stage functionalisation of complex molecules
- Applications for drug/agrochemical discovery & chemical biology

Dr Craig P. Johnston, Royal Society University Research Fellow, University of St Andrews
Dr Christopher Lancefield
University of St Andrews
<table>
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<tr>
<th>Year</th>
<th>Degree</th>
<th>Institution</th>
<th>Supervisor</th>
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<td>2007</td>
<td>MChem</td>
<td>University of Warwick</td>
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<tr>
<td>2011</td>
<td>PhD</td>
<td>Durham University</td>
<td>Dr Ivana Evans</td>
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<td>2011-2012</td>
<td>PDRA</td>
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<td>University of Liverpool</td>
<td>Prof. Matt Rosseinsky</td>
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<tr>
<td>2014-2018</td>
<td>PDRA</td>
<td>University of St Andrews</td>
<td>Prof. John Irvine</td>
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</tbody>
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Dr Julia L. Payne

Batteries  In-situ/operando  Photovoltaics

Reducing/oxidising conditions
Temperature
Current/potential

Operating conditions

New material

Electrochemical performance

Capacity (mA h g⁻¹)

Volume (V)
Dr Marc Reid
University of Strathclyde
Dr Bengt Tegner
Heriot Watt University
Computational Chemistry of Surfaces and Solids

Dr Bengt Tegner
ScotCHEM Recent Appointees Workshop
Dundee V&A
17th June 2019
Research Portfolio
Dr Drew Thomspson
University of Glasgow
Dr Laia Vila Nadal
University of Glasgow
Dr Laia Vilà-Nadal

SELF-ASSEMBLY & PROPERTIES
OF METAL OXIDES
Dr Laia Vilà-Nadal

DIGITAL CHEMISTRY UofGla INITITATIVE: Collaboration with Prof Lee Cronin
Discussion
Garden Group Research Themes

- Renewable Feedstocks
- Polymers
- Sustainability
- Catalysis
- Ligand Design
- Hetero-metallic
- Earth Abundant Metals
Motivation and Overview

Main group catalysts
- different metals for different roles

Efficient catalysis
- renewable resources
- epoxide opening = efficient initiation

Early/late transition metal catalysts
- 2 metals required for catalyst activity
- broad monomer scope

Polymer materials
Initiation mechanisms
- degradation

Ring-opening polymerisation
- homometallic analogues are inactive