University of Glasgow

University of Aberdeen

University of Dundee

ScotCHEM

Recent Appointees Workshop

ECR Flash Presentations

University of Strathclyde Glasgow

University of St Andrews

Heriot-Watt University

The University of Edinburgh

ScotCHEM

Early Career Researchers

ScotCHEM

Dr Graeme Barker

Heriot Watt University

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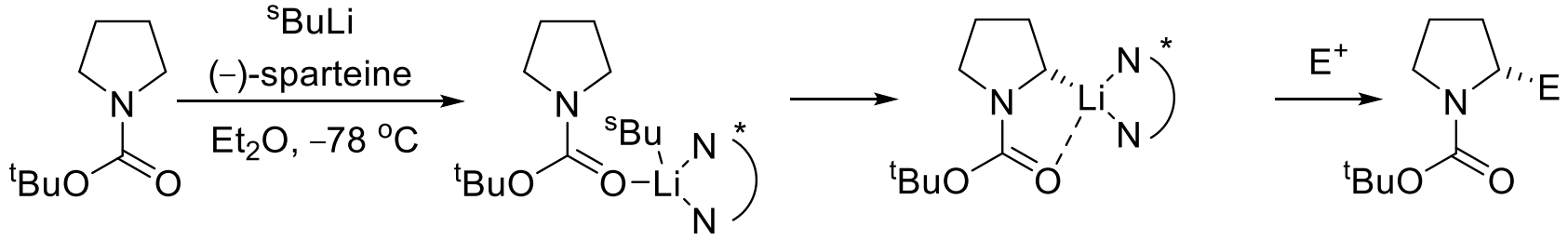
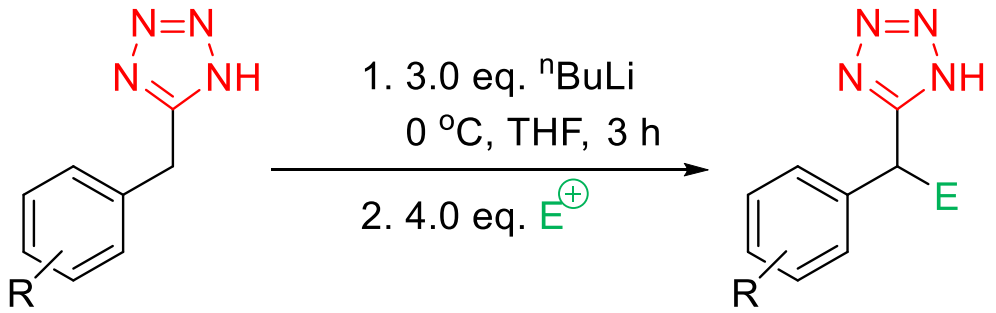
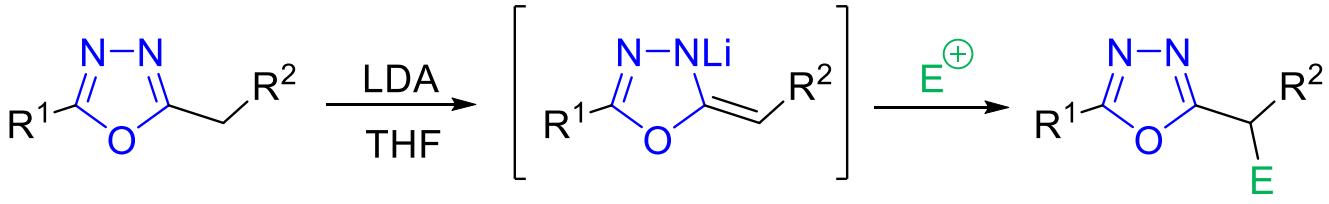
Graeme Barker: Methodology





- 18 Examples
- ≤91% yield
- Important phamaceutical motif

requires –30 °C in batch



usable at rt in flow

- 33 Examples
- ≤100% yield
- Also important pharmaceutical motif

P. Beak *et al.*, *J. Am. Chem. Soc.*, 1991, **113**, 9708

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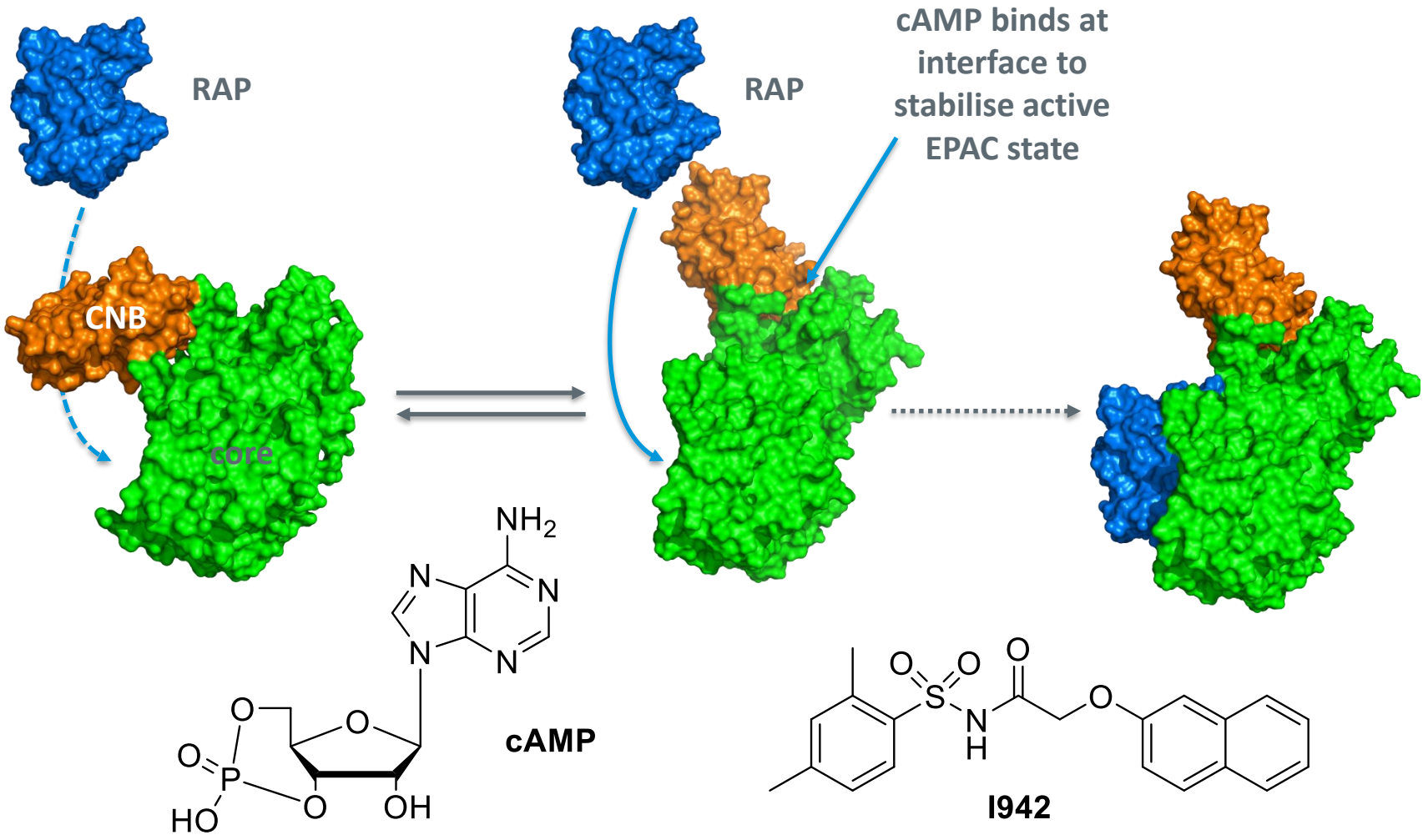
Graeme Barker: MedChem



E. Parnell *et al.*, *Trends Phamacol. Sci.*, 2015, **36**, 203
E. Parnell *et al.*, *Sci. Rep.*, 2017, **7**, 294

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Dr Nicholle Bell

University of Edinburgh

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Dr Damiano Bonaccorso

University of St Andrews

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Dr James Cumby
University of Edinburgh

ScotCHEM

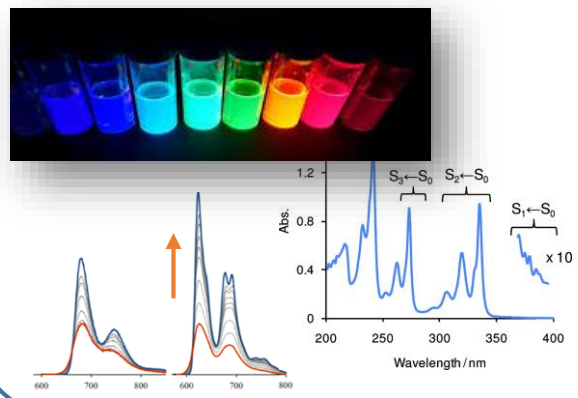
Dr Robert Edkins
University of Strathclyde

Robert Edkins
University of Strathclyde

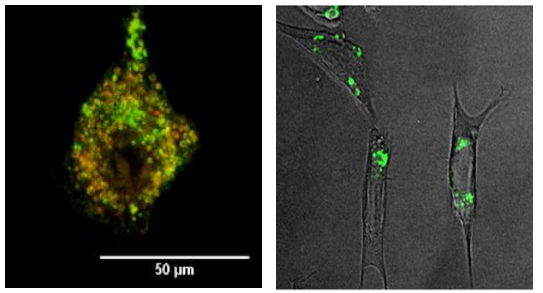
Understanding optical properties of molecules

Design of new molecules for optical applications

Fundamental photophysics

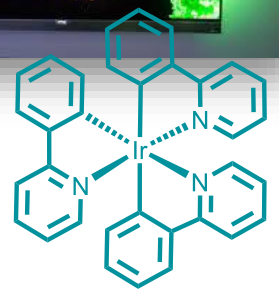


Bioimaging

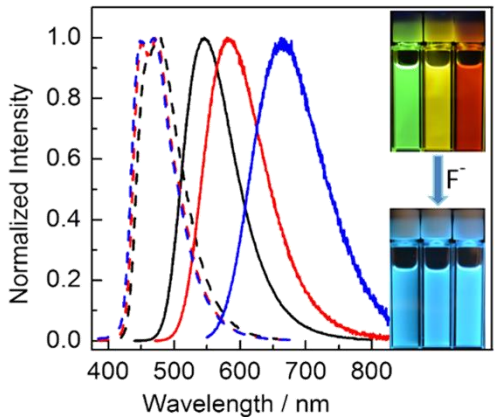


Two-photon, FLIM & STED

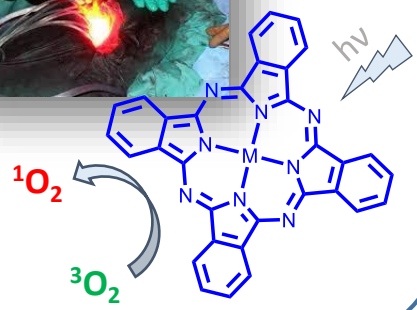
Optoelectronics



Sensing

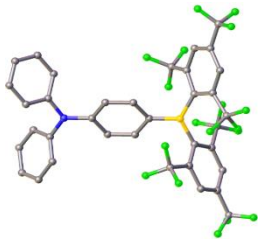


Photodynamic therapy



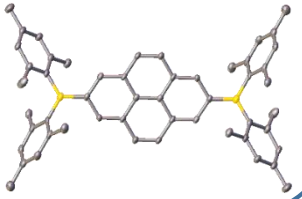
@R_M_Edkins

Triarylboranes



Strong π-acceptors

Reduction to radicals

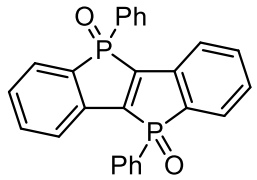


Robert Edkins
University of Strathclyde

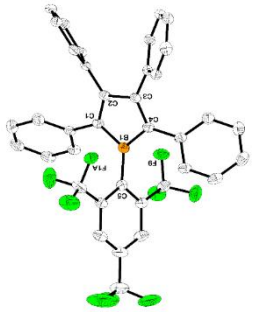
Understanding optical properties of molecules

Design of new molecules for optical applications

Inorganic Heterocycles

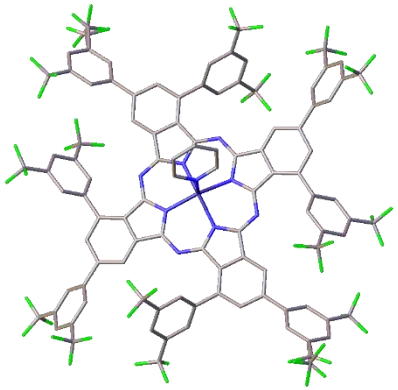


Phospholes



Boroles

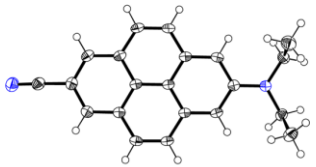
Phthalocyanines

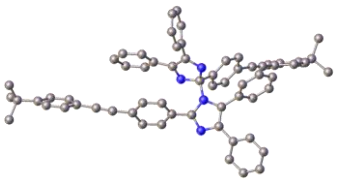


Singlet oxygen photosensitization

Organic chromophores

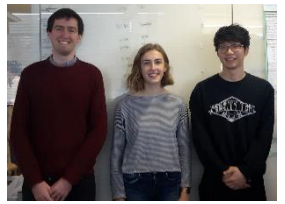
Pyrene derivatives

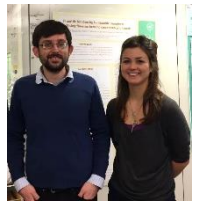




Photochromic imidazoles

Acknowledgements





The group + funding

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University of Edinburgh

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Dr Mairi Haddow

Heriot Watt University

Automated modelling of disordered molecules in crystal structures

Dr Mairi Haddow

Daphne Jackson Trust

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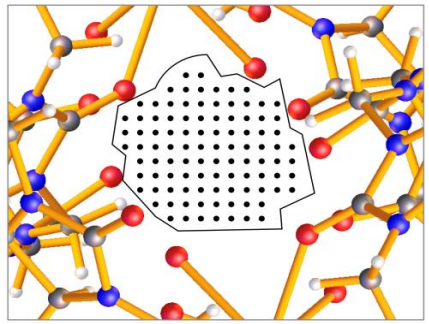
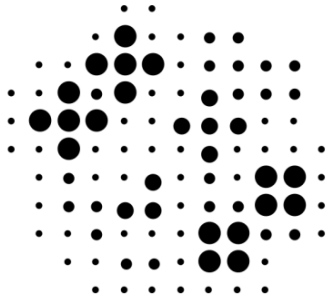
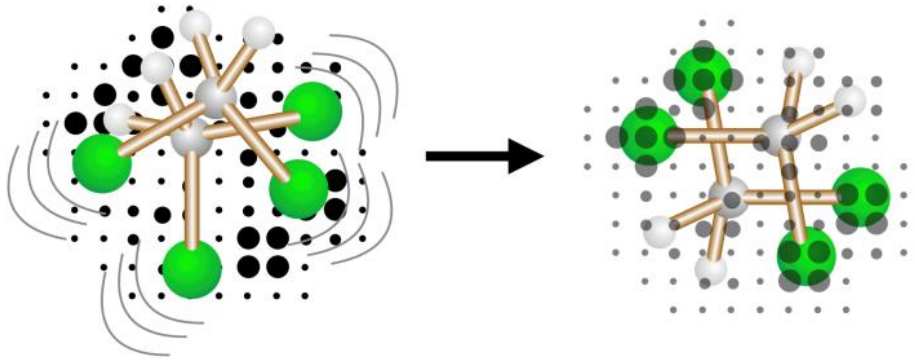
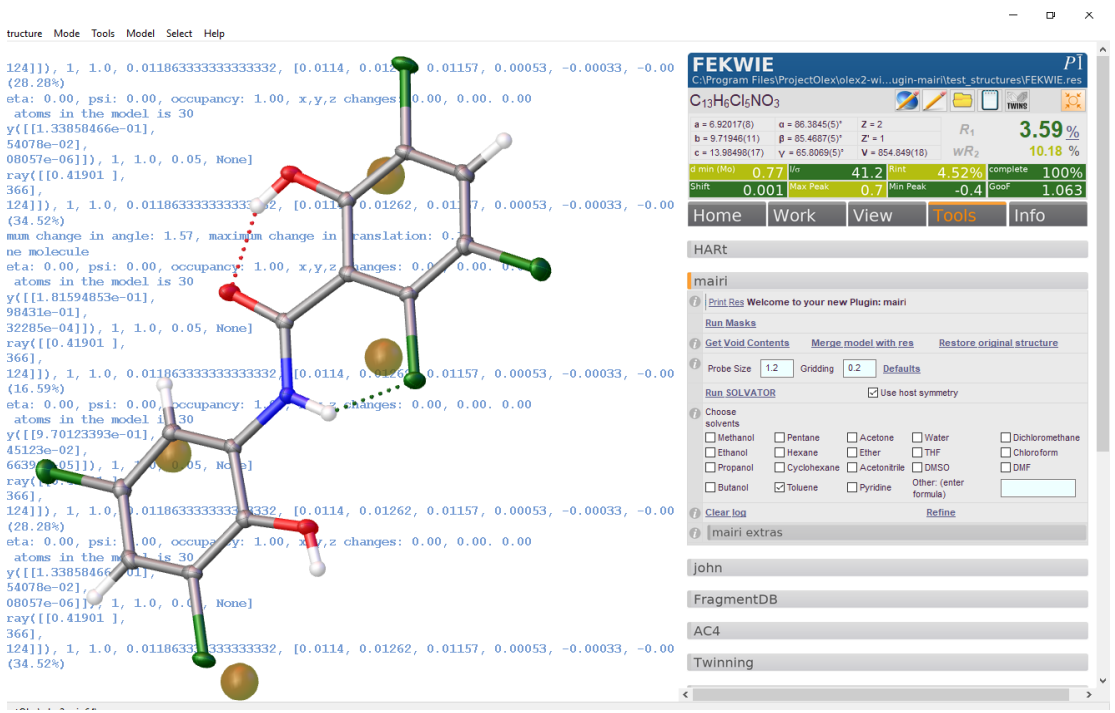
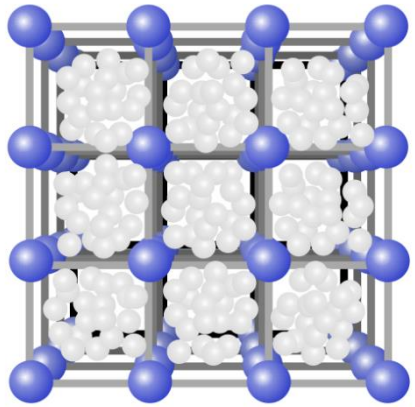
OlexSys











ROYAL SOCIETY OF CHEMISTRY

EPSRC
Engineering and Physical Sciences Research Council

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Dr Gordon Hedley
University of Glasgow

Dr Gordon J. Hedley

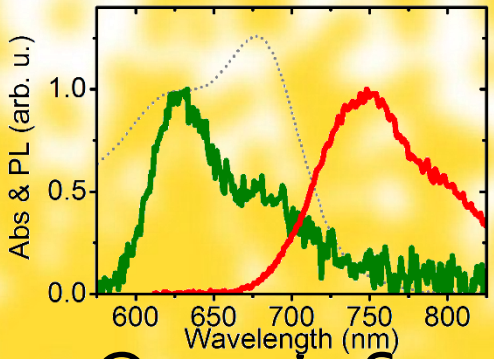
The Hedley Single Molecule Laboratory
University of Glasgow

Single Molecule Spectroscopy

Reducing Concentration

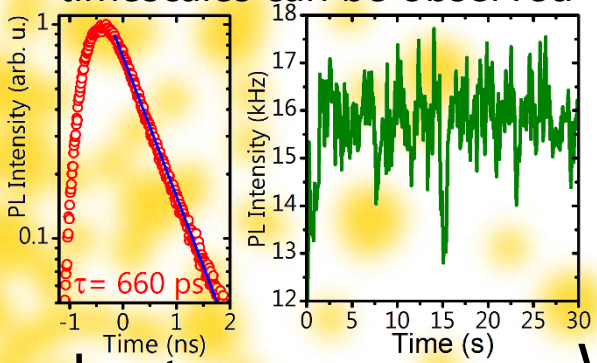
Spectra

The photoluminescence spectra of individual molecules can be measured



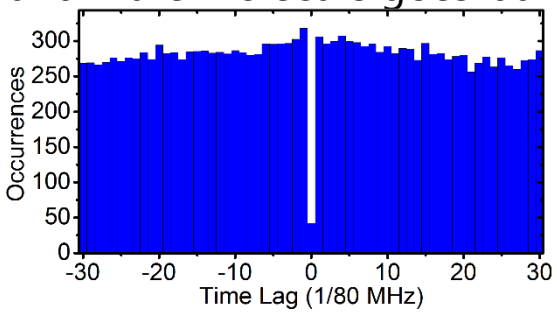
Dynamics

PL dynamics on short (nanosecond) and long (seconds) timescales can be observed



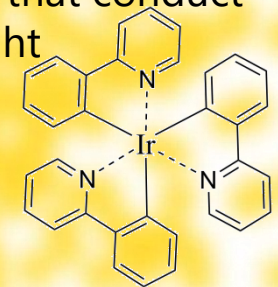
Correlations

Photon correlations tell us how many emitters there are and if the molecule goes 'dark'



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

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Dr Claire Hobday

University of Edinburgh

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Dr Aruna Ivaturi

University of Strathclyde

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Dr Amanda Jarvis
University of Edinburgh

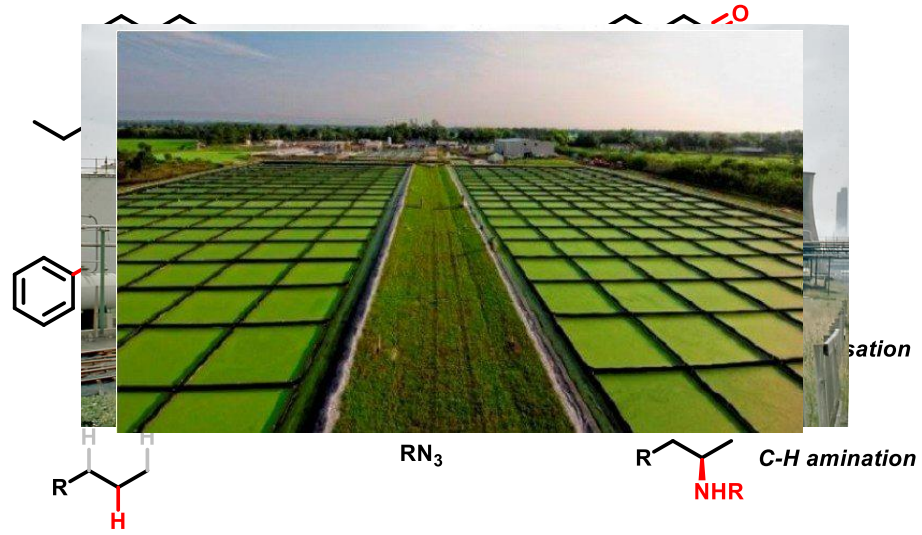
The Jarvis Group

THE UNIVERSITY of EDINBURGH

School of Chemistry, University of Edinburgh, amanda.jarvis@ed.ac.uk

EaStCHEM

Motivation - Sustainable Catalysis:



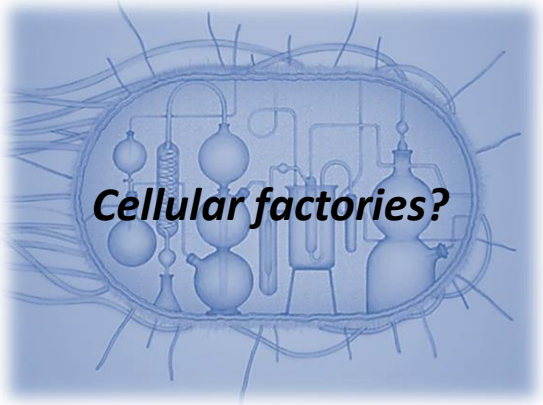
- *Atom economic*
- *Sustainable*
- *Selective functionalisation*
- *Mild conditions*
- *Recovery and reuse of catalyst*

Tool - Artificial metalloenzymes:

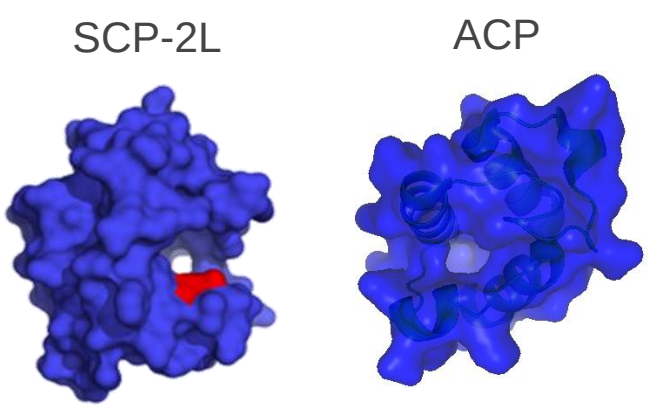
Combining small molecule transition metal catalysts with protein scaffolds.

Benefits of ArMs:

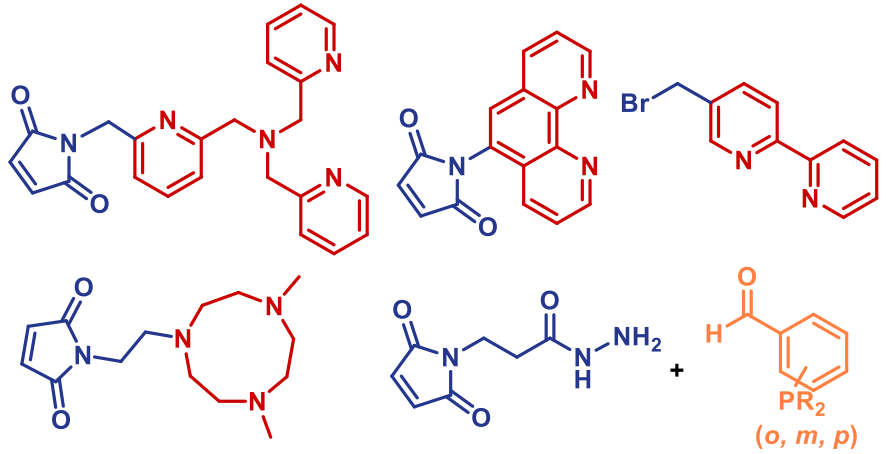
- *Control of substrate orientation – chemo, regio and enantioselective reactions*
- *Evolvable – high throughput optimisation*
- *Possibility of catalysts recovery – biphasic system*
- *Potential for in vivo catalysis, new cascades etc*



Artificial metalloenzyme design



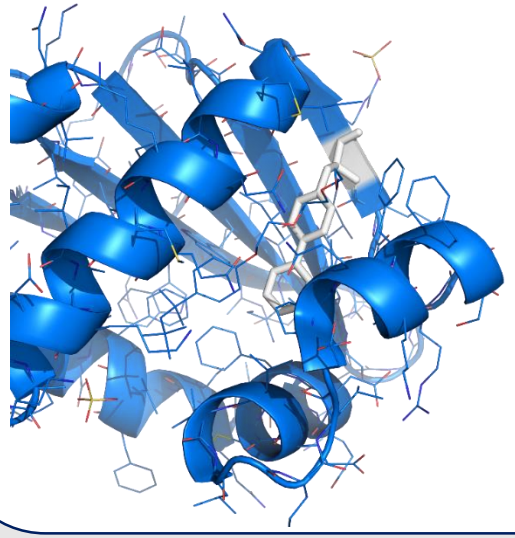
+

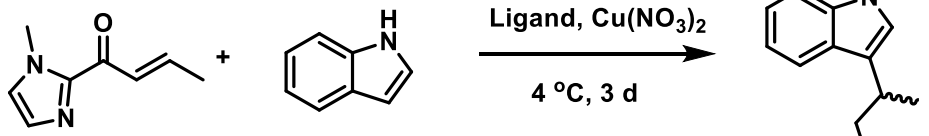


+ Fe, Ru, Pd, Cu, Rh, Mn

= 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

15:85 *e.r.*

Opportunities for collaboration

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

Other applications for these constructs?

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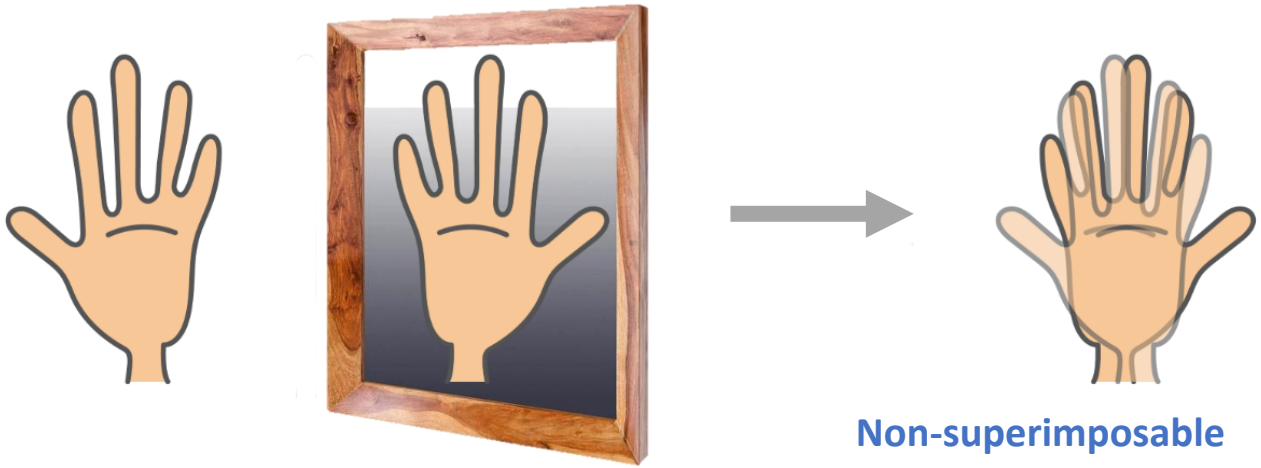
Dr Craig Johnston
University of St Andrews

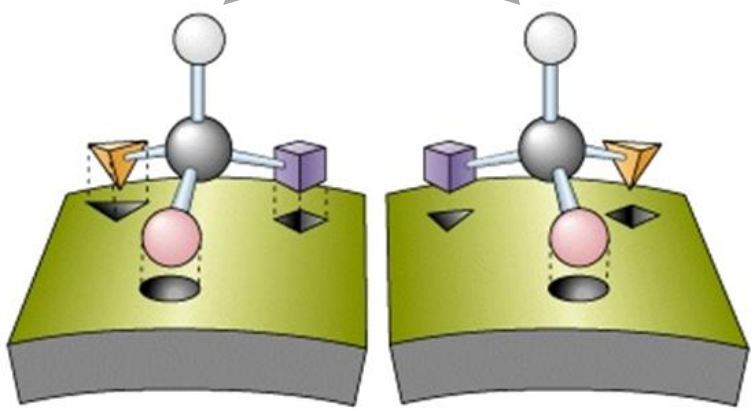
The Importance of Chirality

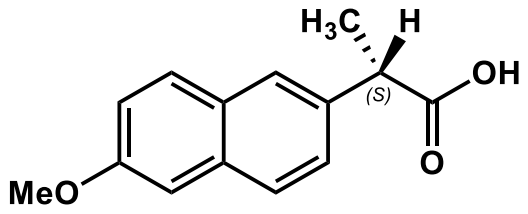


mirror image

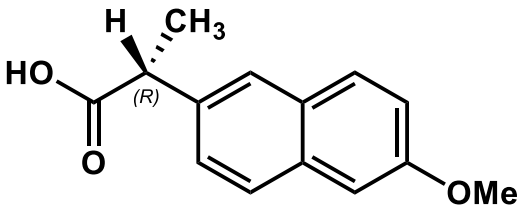
Non-superimposable

enantiomers





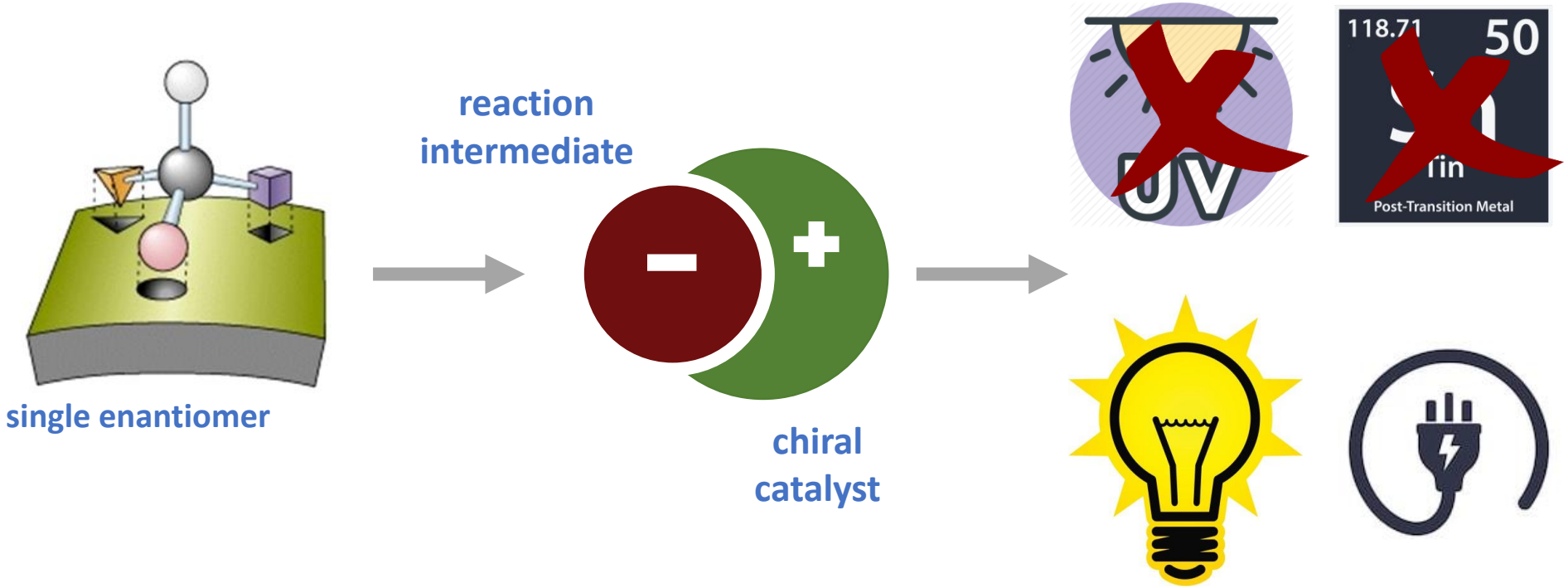
(*S*)-Naproxen
treatment for arthritis



(*R*)-Naproxen
toxic to the liver

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

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

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Dr Christopher Lancefield
University of St Andrews

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Dr Julia Payne

University of St Andrews

Dr Julia L. Payne

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University of St Andrews

SOFCs | Batteries | High Temperature Batteries | Photovoltaics

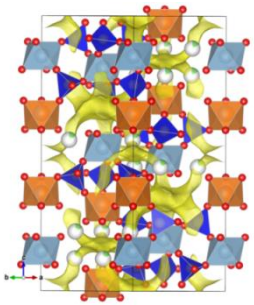
Synthesis | Characterisation | Properties | *In-situ/operando*

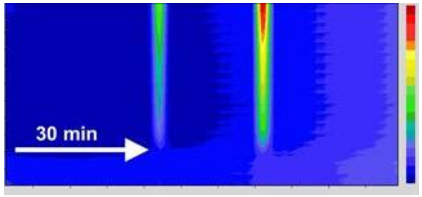
2007	MChem	University of Warwick	
2011	PhD	Durham University	Dr Ivana Evans
2011-2012	PDRA	Durham University	Dr Ivana Evans
2012-2014	PDRA	University of Liverpool	Prof. Matt Rosseinsky
2014-2018	PDRA	University of St Andrews	Prof. John Irvine

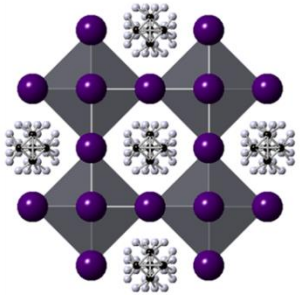
Dr Julia L. Payne

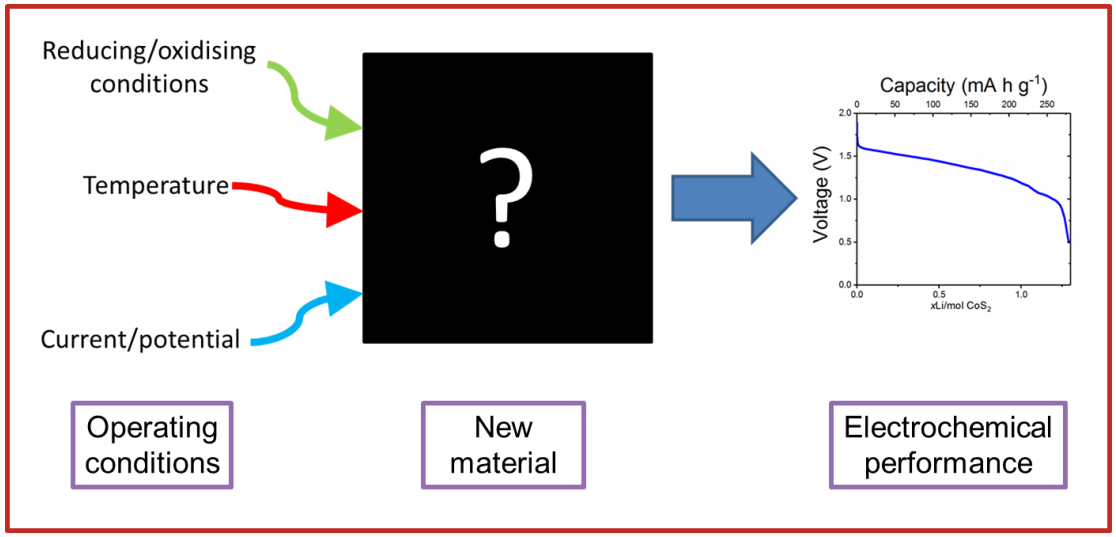
University of St Andrews

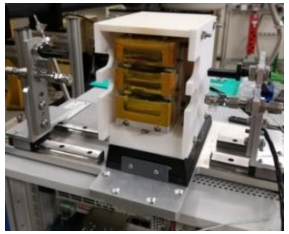
Batteries | *In-situ/operando* | Photovoltaics

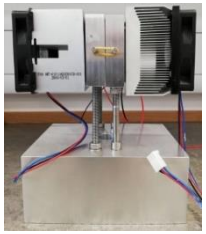


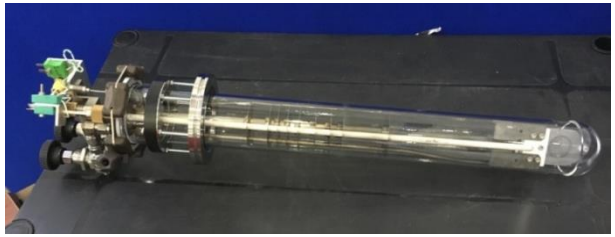












ScotCHEM

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University of Strathclyde

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Dr Bengt Tegner
Heriot Watt University

HERIOT WATT UNIVERSITY

LEADERS IN IDEAS AND SOLUTIONS

Computational Chemistry of Surfaces and Solids

Dr Bengt Tegner

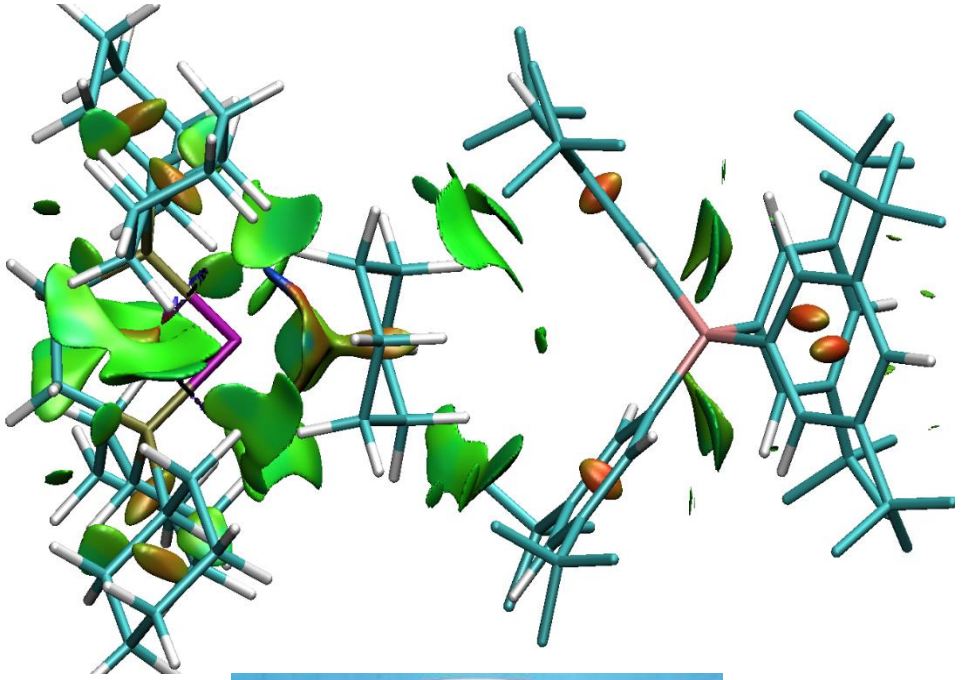
ScotCHEM Recent Appointees Workshop

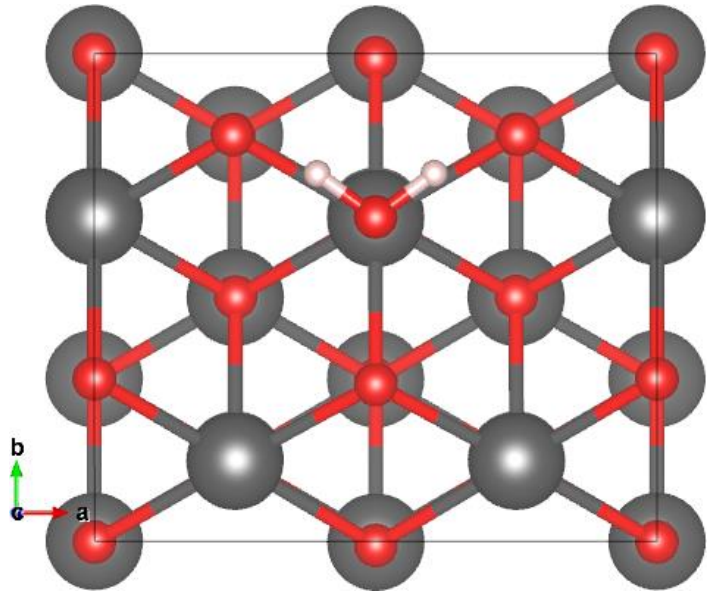
Dundee V&A

17th June 2019

HERIOT WATT UNIVERSITY

Research Portfolio





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Dr Drew Thomspon

University of Glasgow

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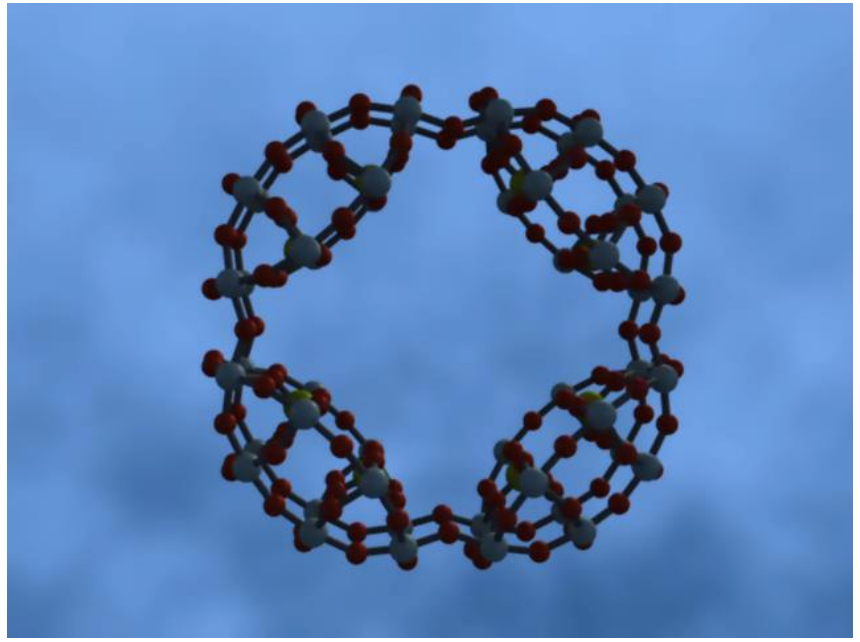
Dr Laia Vila Nadal

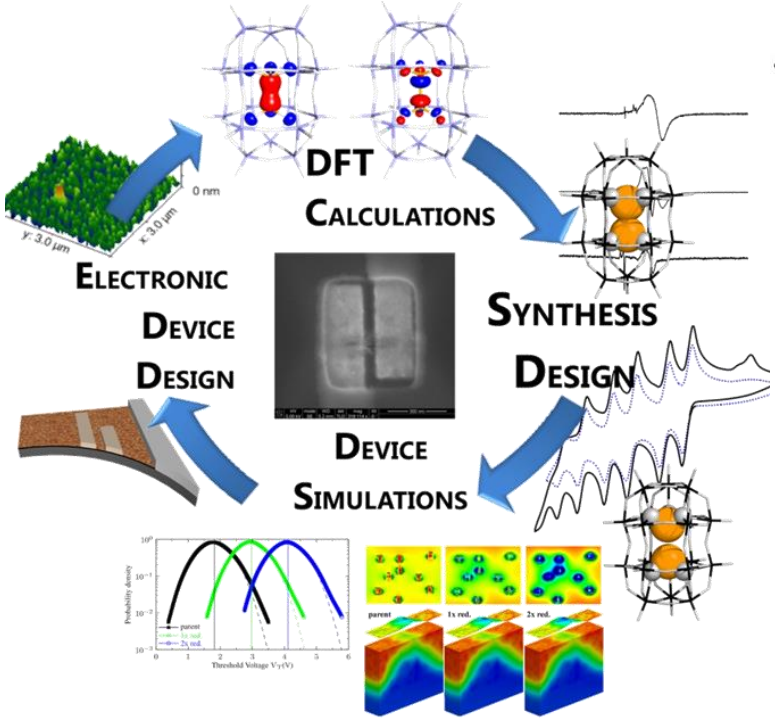
University of Glasgow

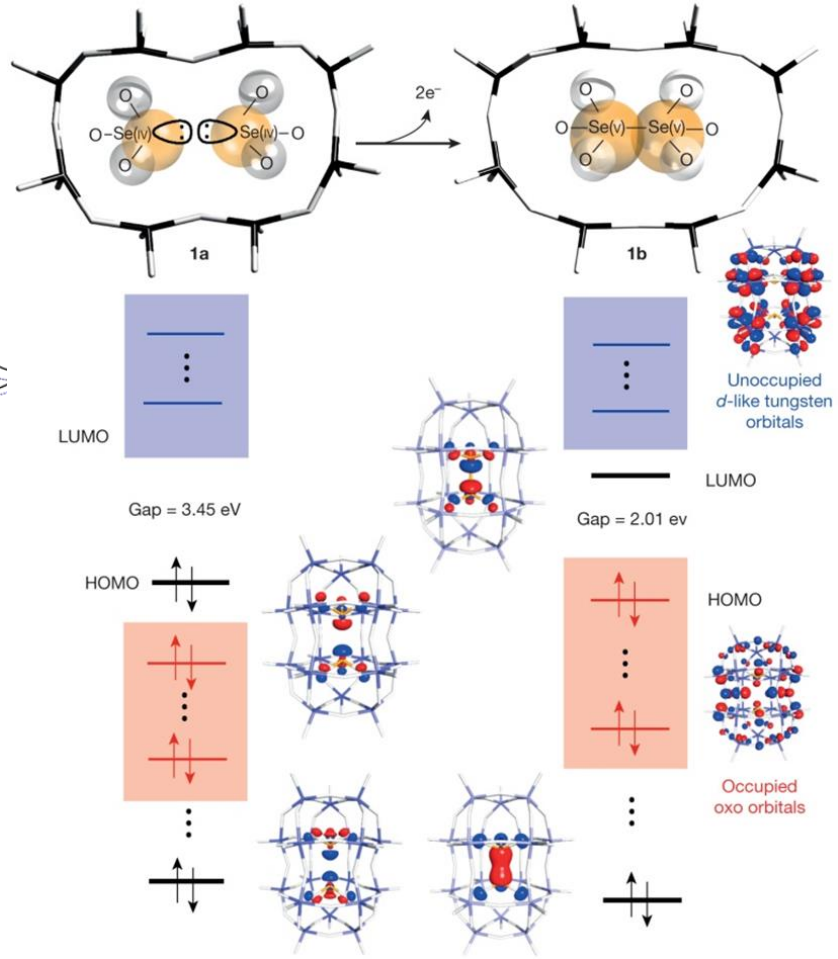
Dr Laia Vilà-Nadal

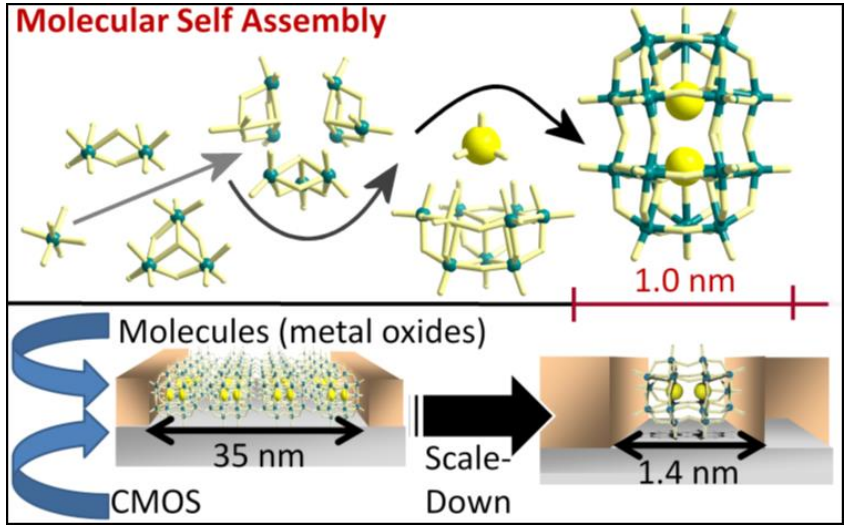
SELF-ASSEMBLY & PROPERTIES OF METAL OXIDES

University of Glasgow





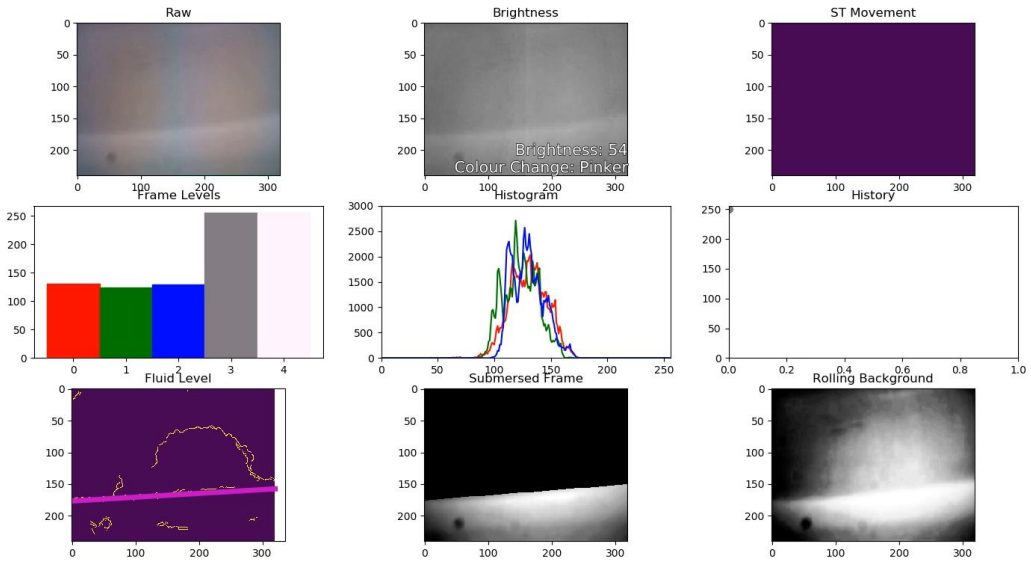


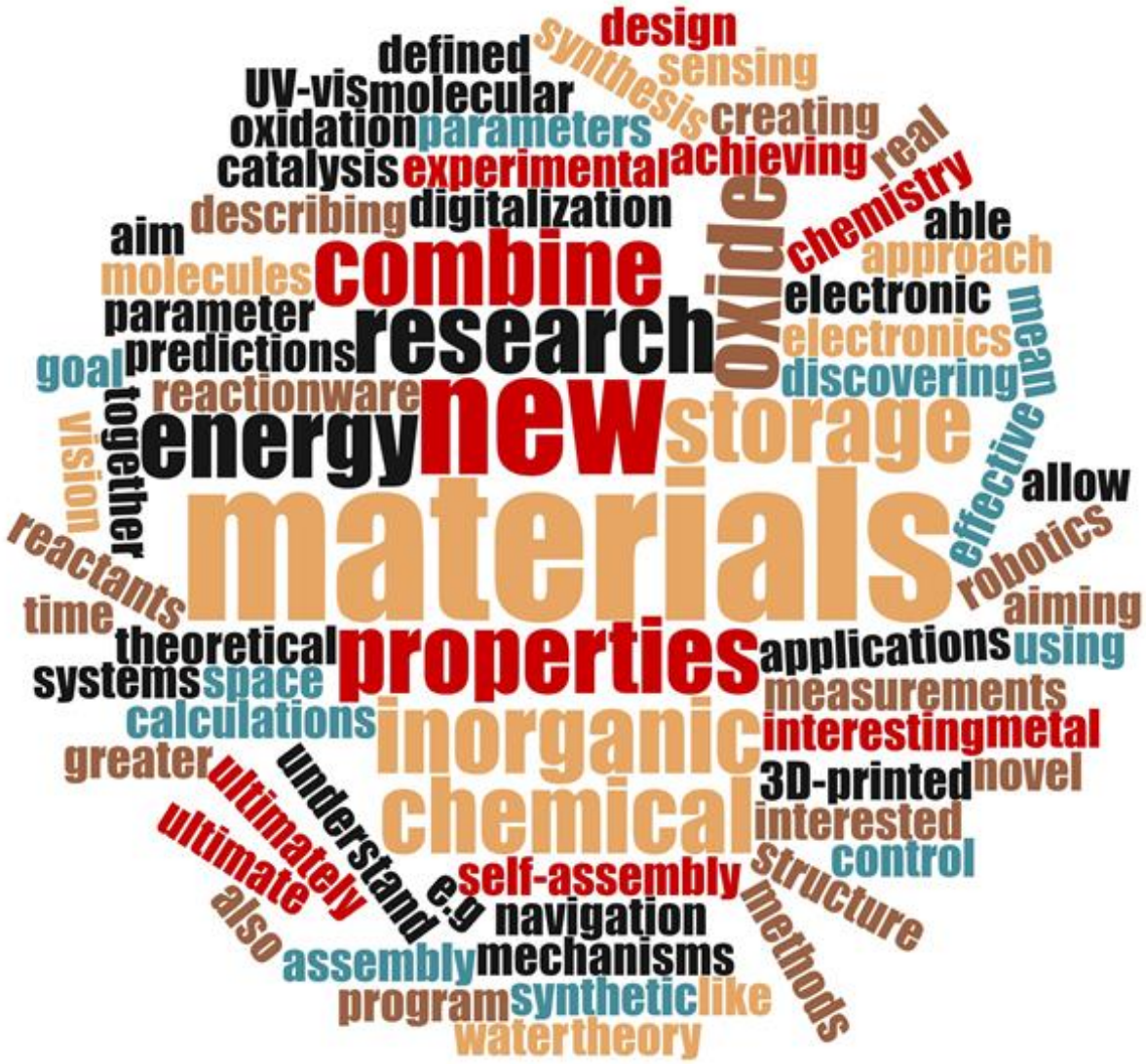


Dr Laia Vilà-Nadal

University of Glasgow

DIGITAL CHEMISTRY UofGla INITITATIVE: Collaboration with Prof Lee Cronin

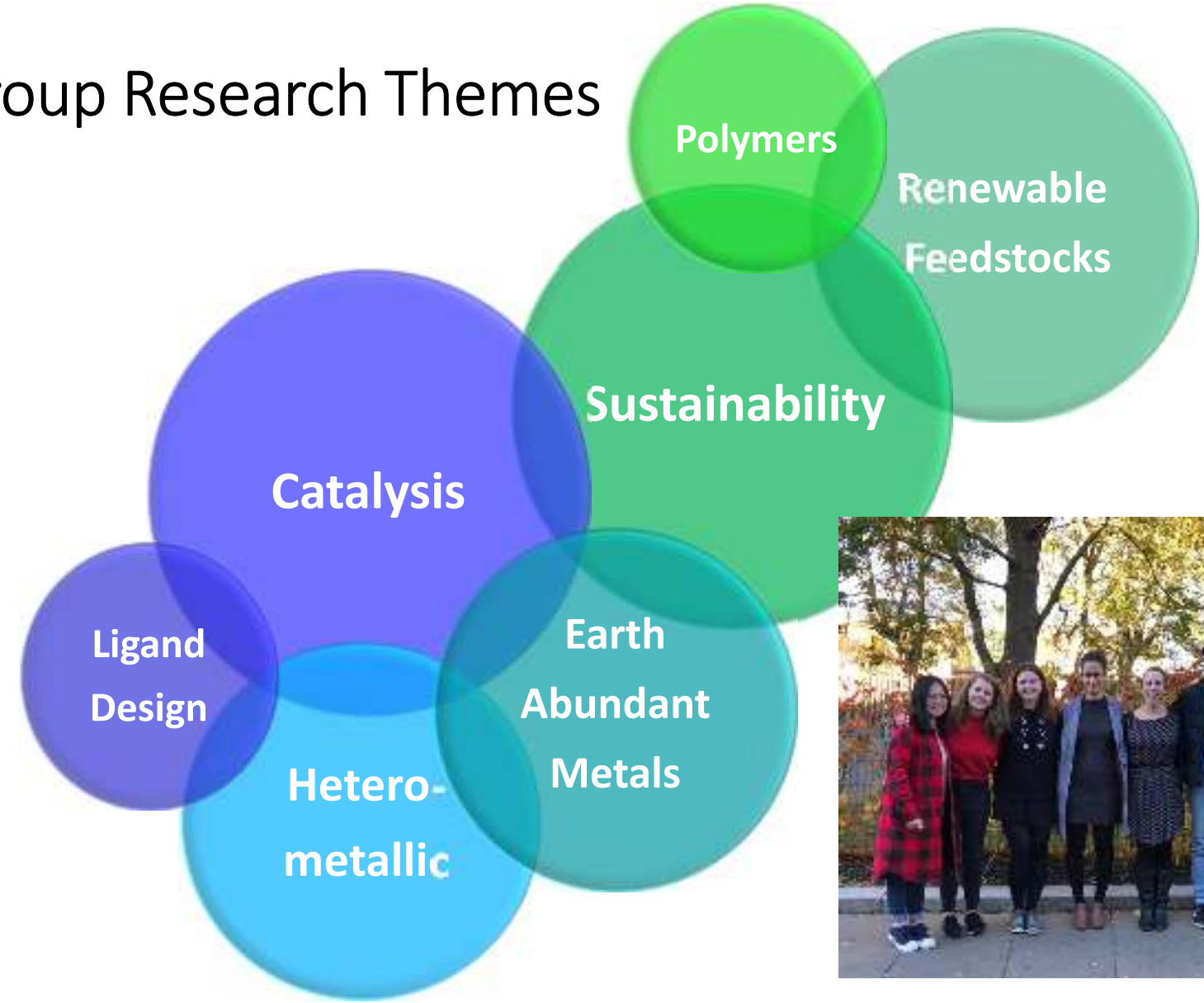




ScotCHEM

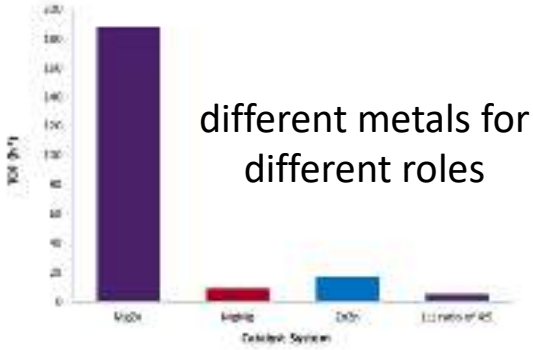
Discussion

Garden Group Research Themes



Motivation and Overview

Main group catalysts



different metals for different roles

efficient catalysis

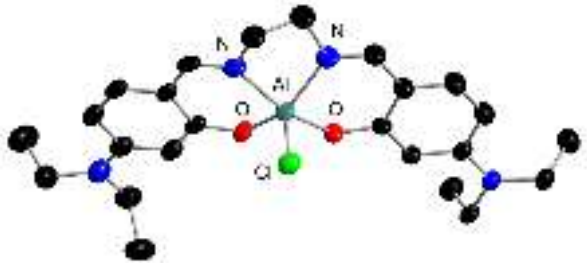
Early/late transition metal catalysts

2 metals required for catalyst activity

renewable resources

polymer materials

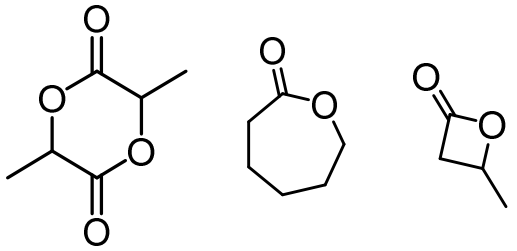
epoxide opening = efficient initiation



Initiation mechanisms

degradation

broad monomer scope



Ring-opening polymerisation