



Inorganic Reaction Mechanisms & Inorganic Biochemistry Discussion Group Meeting

Joint Meeting at the Manchester Institute of Biotechnology from the 15th to 17th of April (2019)

Venue: MIB Lecture Theatre, John Garside Building, 131 Princess Street, Manchester, M1 7DN

Monday the 15th of April

- 12:00 – 13:00 Registration / Tea / Coffee (*Atrium, Manchester Institute of Biotechnology*)
- 13:00 – 13:15 Welcome by the Chairs (Sam de Visser & Nick Le Brun) (*MIB Lecture Theatre*)

Session 1: Sam de Visser (University of Manchester) Chair.

- 13:15 – 14:00 Plenary lecture of Christine McKenzie (University of Southern Denmark, Odense, Denmark), *A Janus-faced iron catalyst. (PL1)*
- 14:00 – 14:20 Sara Kyne (University of Lincoln, Lincoln, UK), *Mechanistic studies of radical reactions: Improving efficiency of chain processes. (OL1)*
- 14:20 – 14:40 James Walton (Durham University, Durham, UK), *Catalytic reaction of organometallic ruthenium complexes. (OL2)*
- 14:40 – 15:00 Jonathan A. R. Worrall (University of Essex, Colchester, UK), *An aromatic dyad motif in dye decolorizing peroxidases has implications for free radical formation and catalysis. (OL3)*
- 15:00 – 15:30 Coffee break (*Atrium*)

Session 2: Sara Kyne (University of Lincoln) Chair.

- 15:30 – 15:50 Marta Chrzanowska (N. Copernicus University, Toruń, Poland), *Substitution behaviour and tuning of $[Ru^{II}(terpy)(N^{\wedge}N)X]^{+2+}$ complexes. (OL4)*
- 15:50 – 16:10 Luisa Ciano (University of York, York, UK), *The molecular basis of polysaccharide cleavage by in lytic polysaccharide monoxygenases. (OL5)*
- 16:10 – 16:30 Callum R. Woolf (University of Bath, Bath, UK), *Iron-catalysed isomerisation of alkenes – exploring reactivity & mechanism through synthesis, spectroscopy & DFT. (OL6)*
- 16:30 – 16:50 M. Qadri E. Mubarak (University of Manchester, Manchester, UK), *Computational modelling on the mechanism of vanadium haloperoxidases. (OL7)*
- 16:50 – 18:15 Poster session and drinks reception (*Atrium*)
- 18:15 – unlimited, socializing

Tuesday the 16th of April

Session 3: Emma Raven (University of Bristol) Chair.

- 09:00 – 09:45 Nyholm Award Lecture by Stephen Mann (University of Bristol, United Kingdom),
Synthetic protobiology: the chemistry of life-like objects. (AL1)
- 09:45 – 09:50 *Nyholm Award Ceremony.*
- 09:50 – 10:10 Lisa Miller (University of York, York, UK),
Antibiotic-functionalised surfaces for the detection of β -lactamases. (OL8)
- 10:10 – 10:30 Samuel M. Neale (Heriot-Watt University, Edinburgh, United Kingdom),
Mechanistic studies into iron-catalysed transfer hydrogenation using amines and boranes.
(OL9)
- 10:30 – 11:00 Coffee break (*Atrium*)

Session 4: Claudia Blindauer (University of Warwick) Chair.

- 11:00 – 11:20 Aidan R. McDonald (Trinity College Dublin, Dublin, Ireland),
Mimicking class Ib Mn_2 -ribonucleotide reductase: Mn^{II}_2 complexes and their reaction with superoxide. (OL10)
- 11:20 – 11:40 Sophie Bennett (University of East Anglia, Norwich, UK),
*Copper centre biogenesis in the nitrous oxide reductase of *Paracoccus denitrificans*.* (OL11)
- 11:40 – 12:00 Danila Gasperini (University of Bath, Bath, UK),
Seeking heteroatom rich compounds; iron catalysed efficient heterodehydrocoupling of N-Si bond followed by desilacoupling to N-B linkages. (OL12)
- 12:00 – 12:20 Jason Lynam (University of York, York, UK),
Probing manganese-catalysed C-H functionalisation with time-resolved infra-red spectroscopy. (OL13)
- 12:20 – 15:00 Lunch break, Poster Session and Network opportunities (*Atrium*)
- 13:30 – 14:30 Committee meetings of IRMG and IBDG
- 13:30 – 14:30 *Tour through MIB labs (Derren Heyes).*
- 15:00 – 15:35 Coffee break (*Atrium*)

Session 5: Grace Morgan (University College Dublin) Chair.

- 15:35 – 15:55 Justin Bradley (University of East Anglia, Norwich, UK),
Mapping iron transit through ferritins. (OL14)
- 15:55 – 16:15 Galvin Leung (University of Leicester, Leicester, UK),
Precise determination of heme binding affinity in proteins. (OL15)
- 16:15 – 17:00 Plenary talk by Francesca Paradisi (University of Nottingham, Nottingham, UK),
Carbene ligand to replace histidine in cupredoxin protein scaffolds. (PL2)

Wednesday the 17th of April

Session 7: Nick Le Brun (University of East Anglia) Chair.

- 09:00 – 09:45 Plenary Lecture by Miquel Costas (University of Girona, Girona, Spain),
Fe^V complexes of relevance in enzymology and organic synthesis. (PL3)
- 09:45 – 10:05 Charlène Esmieu (University of Toulouse, Toulouse, France),
Effect of the N-truncation of Aβ peptides on the ROS production by their copper complexes – Friends or enemies? (OL16)
- 10:05 – 10:25 Hazel Girvan (University of Manchester, Manchester, UK),
Mechanistic and structural studies on members of the CYP152 peroxygenase family of cytochromes P450. (OL17)
- 10:25 – 11:00 Coffee break (*Atrium*)

Session 8: Jonathan Worrall (University of Essex) Chair.

- 11:00 – 11:20 Megan Greaves (University of Strathclyde, Glasgow, UK),
Probing the Mechanism of Oxidative Addition of Alkyl Substrates to Ni⁰. (OL18)
- 11:20 – 11:40 Amanda Jarvis (University of Edinburgh, Edinburgh, UK),
Artificial metalloenzymes for hydrocarbon functionalisation. (OL19)
- 11:40 – 12:00 Ulrich Hintermair (University of Bath, Bath, UK),
Is there an alternative to the Haber-Bosch process? An ab-initio analysis of the catalytic oxidation of nitrogen. (OL20)
- 12:00 – 12:20 Sophie Kendall-Price (University of Oxford, Oxford, UK),
Combining solution and single crystal IR spectroelectrochemistry reveals details of the [NiFe] hydrogenase catalytic cycle. (OL21)
- 12:20 Closing ceremony and final comments by the Chairs.

Summary:

Award Lecture:	Stephen Mann (University of Bristol, Bristol, UK).
Plenary talk 1:	Christine McKenzie (University of Southern Denmark, Odense, Denmark)
Plenary talk 2:	Francesca Paradisi (University of Nottingham, Nottingham, UK)
Plenary talk 3:	Miquel Costas (University of Girona, Girona, Spain)
Oral presentation 1:	Sara Kyne (University of Lincoln, Lincoln, UK)
Oral presentation 2:	James Walton (Durham University, Durham, UK)
Oral presentation 3:	Jonathan A. R. Worrall (University of Essex, Colchester, UK)
Oral presentation 4:	Marta Chrzanowska (N. Copernicus University, Toruń, Poland)
Oral presentation 5:	Luisa Ciano (University of York, York, UK)
Oral presentation 6:	Callum Woof (University of Bath, Bath, UK)
Oral presentation 7:	M. Qadri E. Mubarak (University of Manchester, Manchester, UK)
Oral presentation 8:	Lisa Miller (University of York, York, UK)
Oral presentation 9:	Samuel M. Neale (Heriot Watt University, Edinburgh, UK)
Oral presentation 10:	Aidan McDonald (Trinity College Dublin, Dublin, Ireland)
Oral presentation 11:	Sophie Bennett (University of East Anglia, Norwich, UK)
Oral presentation 12:	Danila Gasperini (University of Bath, Bath, UK)
Oral presentation 13:	Jason Lynam (University of York, York, UK)
Oral presentation 14:	Justin Bradley (University of East Anglia, Norwich, UK)
Oral presentation 15:	Galvin Leung (University of Leicester, Leicester, UK)
Oral presentation 16:	Charlène Esmieu (University of Toulouse, Toulouse, France)
Oral presentation 17:	Hazel Girvan (University of Manchester, Manchester, UK)
Oral presentation 18:	Megan Greaves (University of Strathclyde, Glasgow, UK)
Oral presentation 19:	Amanda Jarvis (University of Edinburgh, Edinburgh, UK)
Oral presentation 20:	Ulrich Hintermair (University of Bath, Bath, UK)
Oral presentation 21:	Sophie Kendall-Price (University of Oxford, Oxford, UK)

Poster presentations:

- P1: Felicia Ejia (University of Lagos, Lagos, Nigeria)
- P2: Melissa Stewart (University of East Anglia, Norwich, UK)
- P3: Marta Chrzanowska (Copernicus University, Toruń, Poland)
- P4: Manel Martínez (University of Barcelona, Barcelona, Spain)
- P5: Niting Zeng (University of Manchester, Manchester, UK)
- P6: Yen-Ting Lin (University of Manchester, Manchester, UK)
- P7: Miron Leanca (University of Manchester, Manchester, UK)
- P8: Alex Miller (Liverpool John Moores University, Liverpool, UK)
- P9: Emilie F. Gérard (University of Manchester, Manchester, UK)
- P10: Adam Barrett (University of Bath, Bath, UK)
- P11: Oliver Manners (University of Manchester, Manchester, UK)
- P12: David McLaughlin (University College Dublin, Dublin, Ireland)
- P13: Mary Ortmayr (University of Manchester, Manchester, UK)
- P14: Mads Sondrup Møller (University of Southern Denmark, Odense, Denmark)
- P15: Line Sofie Hansen (University of Southern Denmark, Odense, Denmark)
- P16: Tobias Hedison (University of Manchester, Manchester, UK)
- P17: Arron Burnage (Heriot-Watt University, Edinburgh, UK)
- P18: Amirah Kamaruddin (University of Manchester, Manchester, UK)
- P19: Sidra Ghafoor (Government College University, Faisalabad, Pakistan)
- P20: Sangita Das (Durham University, Durham, UK)
- P21: David Collison (University of Manchester, Manchester, UK)
- P22: Sultan Alkaabi (University of Manchester, Manchester, UK)