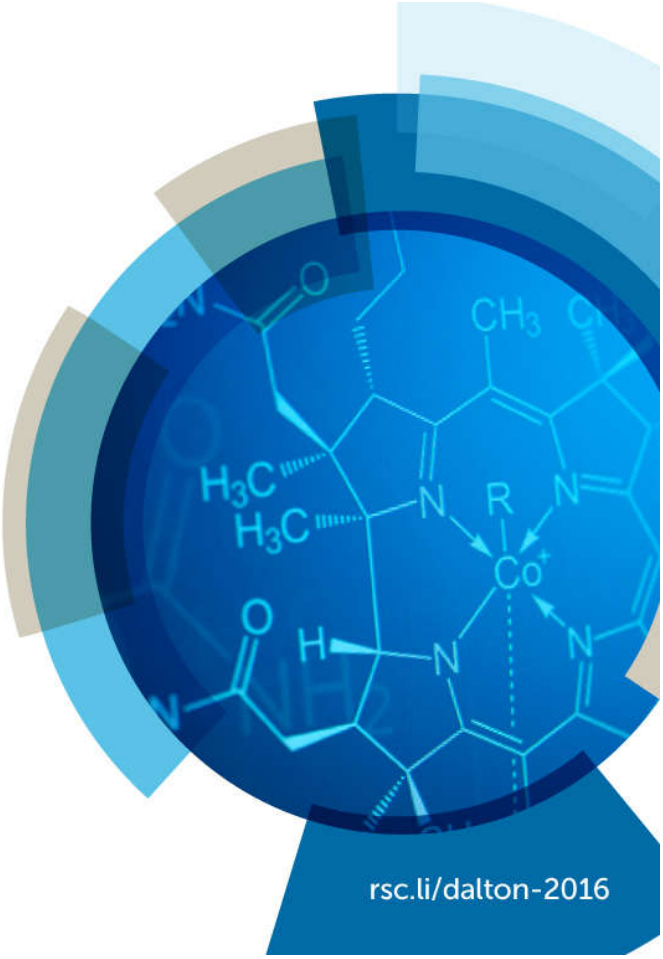
ROYAL SOCIETY OF CHEMISTRY

Dalton 2016

Joint Interest Groups Meeting



29-31 March 2016
University of Warwick, UK

Programme and Oral Abstracts

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John Dalton, F.R.S

Tuesday 29th March 2016

13.30 – 13.45 Welcome and Introduction: David Cole-Hamilton (**Lecture Theatre L3**)

13.45 – 14.30 **Todd Marder**, *Julius-Maximilians-Universität Würzburg* Synthesis and Photophysical Properties Rhodacycles Formed via Unusual Diyne Couplings

Plenary lecture (L3) Session Chair: Mike Hill

14.30 – 15.15 **Eric Rivard**, *University of Alberta* Using Ligand Design and Donor-acceptor Stabilization to Access New Bonding Modes and Functional Nanodimensional Materials

15.15 – 15.40 Tea/Coffee

Parallel session 1

	Coordination & Organometallic	**Main Group**	**Inorganic Biochemistry**	**Reaction Mechanisms**	**5+5+5 Headline**
Room	L3	L4	B202	B204/5	L5
Chair	Patrick McGowan	Jose Goicoechea	Alison Parkin	Sam de Visser	David Cole-Hamilton
15.40-16.00	**Mark Chadwick** *University of Oxford* Organometallic chemistry in the solid state: isolating a sigma-pentane compound	**Christian Sindlinger** *University of Oxford* Organotin(IV) di- and trihydrides as precursors for low-oxidation state organotin chemistry by dihydrogen release	**Anna Peacock** *University of Birmingham* IBDG Young Investigator Award Lecture: Advancing metalloprotein design for new functions and applications	**Stuart MacGregor** *Heriot-Watt University* Modelling Organometallic Structure and Reactivity in the Solid State	**Laurel Schafer** *University of British Columbia* N,O-chelates becoming unhinged. New perspectives in metal-ligand cooperativity
16.00-16.20	**Thomas Pugh** *University of Manchester* Magneto-Structural Correlations in Dysprosium Single-Molecule Magnets	**Michael Cowley** *University of Edinburgh* Synthesis and reactivity of phosphinidene boranes		**Tomas Belderrain** *CIQSO. Universidad de Huelva* Mechanistic Study of C-N Bond Formation Reaction Catalysed By a NHC- Nickel(0) Complex	**Michael Wolf** *University of British Columbia* Controlling Optical Properties of Conjugated Oligomers Using Metal and Main Group Chemistry
16.20-16.40	**Pierre Kennepohl** *University of British Columbia* Reexamining Oxidation States in Transition Metal p-complexes: Implications for Reactivity	**Merle Arrowsmith** *Universität Würzburg* Small molecule activation by CAAC-stabilised low-valent boron species	**Lars Jeuken** *University of Leeds* Proton-pumping and hydrogen oxidation in respiration	**Lena Albers** *University of Edinburgh* Cationic Rearrangements in Polysilanes - Subtle Capture of Intermediates	**Paul Ragogna** *University of Western Ontario* Four-membered pnictogen-chalcogen rings: Synthesis and chemistry
16.40-17.00	**Heikki Tuononen** *University of Jyväskylä* Synthesis and characterization of a new air stable 1,2,4-triazinyl radical and its coordination complexes	**Thomas Robinson** *University of Oxford* Small Molecule Activation at a Geometry-Constrained Phosphorus Centre	**Philip Ash** *University of Oxford* Differences in inhibition of NiFe hydrogenases studied by protein film infrared electrochemistry	**Lucy Milner** *University of York* Outer-Sphere Electrophilic Fluorination (OSEF) of Organometallic Fragments	**Webster Santos** *Virginia Tech* Towards Borylation Reactions in Aqueous Medium
17.00-17.20	**Benjamin Clough** *University of Oxford* Synthesis and reactivity of titanium borylimido compounds	**Peter Portius** *University of Sheffield* Nitrogen-rich complexes of p-block elements: Highly endothermic polytetrazolates and polyazides	**Luisa Ciano** *University of York* The molecular basis of polysaccharide cleavage by lytic polysaccharide monooxygenases	**Amy Ruddlesden** *University of York* Enhancing NMR: Development of Efficient Polarisation Transfer Catalysts	**Angela Casini** *Cardiff University* "Gold-finger" domains formation: implications for the use of gold compounds in therapy

Tuesday 29th March 2016 (ctd.)

Plenary Lecture (L3) Session chair: Manfred Bochmann

17.30 – 18.15 **Jonas Peters**, *California Institute of Technology* Synthetic Single-site Iron Nitrogenases

18.30 - 19.30 Dinner (Rootes Restaurant)

19.30 – 22.00 Poster session (Sir Geoffrey Wilkinson Dalton Poster Competition) – Physics and Science Concourse

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Wednesday 30th March 2016

Plenary Lectures (L3) Session chair: Patrick McGowan

9.00 – 9.45 **Pedro Pérez**, *Universidad de Huelva* Overcoming the Alkane Inertness toward C-H Functionalization

9.45 – 10.30 **Martha Greenblatt**, *Rutgers* Designing Polar and Magnetic Oxides in the A2BB'O6-Type Corundum Derivatives

10.30 – 10.55 Tea/Coffee

Wednesday 30th March 2016 (ctd.)

Parallel session 2 (5+5+5 contributions are marked with an★)

	Coordination & Organometallic	Coordination & Organometallic (2)	Main Group	Inorganic Biochemistry	Reaction Mechanisms	Engagement
Room	L3	L5	L4	B202	B204/5	B201
Chair	TBA	Jason Love	Charlie O'Hara	Jon Worrall	Stuart MacGregor	
10.55-11.15	**Bradley Holliday** ★ *UT at Austin* Rhenium complexes and conducting metallopolymers for electrocatalytic CO_2 reduction	**Alexander Romanov** *University of East Anglia* Design of Copper and Gold Carbene Complexes for Fabrication of Highly Efficient Organic Light-Emitting Diodes	**Victoria Greenacre** *University of Sussex* Ruthenaphosphaalkenyls – their structure and ambiphilic reactivity	**Amira Ksibe** *University of Warwick* Monitoring conformational changes for Zur, a Zn(II) metalloregulatory protein from Synechococcus sp. WH8102	**Jennifer Love** *University of British Columbia* Studies towards Pt-catalyzed activation of methane	
11.15-11.35	**Manfred Bochmann** *University of East Anglia* New Gold(III) Chemistry: From Structure and Bonding to Photoluminescence and Anti-Cancer Activity	**Arnaud Thevenon** *Imperial College London* Structure-Activity Relationships for Macrocyclic Dinuclear Zinc Complexes for Polymerization: Importance of the Catalyst Structure	**Etienne Brouillet** *University of Strathclyde* Donor Controlled Cation Aggregation in Magnesium Aluminates for Rechargeable Battery Electrolytes	**Erin Dodd** *University of East Anglia* Iron Sulfur cluster nitrosylation mechanism in NsrR: mechanisms of nitrosylation in an NO regulatory protein	**Manuel Martinez** *Universitat de Barcelona* Kinetico-mechanistic studies on substitution reactions on Co(III) and Ru(II) complexes with nucleosides and nucleotides at physiological pH	**Dominic McDonald** *Programme Manager for Outreach, RSC* Challenging Attitudes: Engaging the Public with Chemistry
11.35-11.55	**David Mills** *University of Manchester* Thorium(III) Small Molecule Activation Chemistry	**Gavin Craig** *University of Glasgow* Field-induced slow magnetic relaxation in a mononuclear Mn(III) complex: An ambient and high pressure study	**Alexander Ried** *University of Nottingham* The Stabilisation of Magnesium Complexes using Sterically Demanding N-Donor Ligands	**Justin Bradley** *University of East Anglia* A Ferritin Optimized for Iron Oxidation not Storage	**James Pankhurst** *University of Edinburgh* Earth-abundant mixed-metal systems for hydrocarbon oxidation catalysis	
11.55-12.15	**Fabrizio Ortu** *University of Manchester* Synthetic, Physical and Theoretical Investigation of Lanthanide-Radical Complexes	**Tim Shuttleworth** *University of Bristol* "Proton shuttling" Pyridylphosphines for Methoxycarbonylation	**David Pugh** *University of Southampton* Coordination chemistry of s-block cations with soft donor macrocycles	**Debbie Crans** ★ *Colorado State University* Speciation is central for the mode of action of metal-based drugs	**Einas Abood** *Newcastle University* Polymer Immobilised Ionic Liquid Phase (PIILP) Stabilised Pd-Nanoparticles: Synthesis and Applications in Catalysis	
12.15-12.35	**Joy Farnaby** *Imperial College London* Multi-metallic f-element complexes with redox-active ligands	**Owen Metters** *University of Bristol* Advances in Transition Metal Frustrated Lewis Pair Chemistry	**Simon Aldridge** ★ *University of Oxford* Bond Activation by Highly Reactive Low-valent Germanium Complexes	**Tim Storr** ★ *Simon Fraser University* Targeting Small-Molecules to Treat Alzheimer's Disease	**Adrian Chaplin** *University of Warwick* Preparation and reactivity of $[M(PtBu_3)_2]^+$ (M = Pd, Pt)	**Sarah Newton** European Young Chemists' Network

Wednesday 30th March 2016 (ctd.)

Plenary Lectures (L3) Session chair: Anne-Katrin Duhme-Klair

12.35 – 13.00 Flash Poster Presentations by Poster Prize Winners and Runner-ups

13.00 – 14.00 Lunch (Rootes Restaurant) and poster browsing

Plenary Lectures (L3) Session chair: Robert Mulvey

14.00 – 14.45 **Chris Barnard**, *Johnson-Matthey* Collaborating with the Pharmaceutical Industry - views of a middle man!

14.45 – 15.30 **Claire Carmalt**, *UCL* Sustainable manufacturing of functional materials

15.30 – 15.55 Tea/Coffee

Parallel session 3

	Coordination & Organometallic	Main Group	Inorganic Biochemistry	Reaction Mechanisms	Solid State
Room	L3	L4	L5	B204/5	B202
Chair	Richard Layfield	Ruth Webster	Jon McMaster	Philip Mountford	Emma McCabe
16.00-16.20	**Nikolaos Tsoureas** *University of Sussex* Steric Control of Redox Events in Organo-Uranium Chemistry	**Huayi Fang** *Max Planck Institute for Chemical Energy Conversion* Synthesis and Reactivity Studies of Corrole Germanium Anion, Radical and Cation	**Gabriele Wagner** *University of Chester* New platinum oxadiazoline complexes with antiproliferative properties	**Andrew Weller** ★ *University of Oxford* Metal Catalyzed Amine– and Phosphine–Borane Dehydropolymerisation. Control Through Catalyst Design	**Ross Forgan** *University of Glasgow* Enhancing Stability and Reactivity of Zr Metal-Organic Frameworks
16.20-16.40	**Lucy Wilson** *Imperial College London* Linear, branched and cyclic $Ru(dppe)_2(-C{\equiv}C-)_2$ systems for molecular electronics	**Ulrich Siemeling** *University of Kassel* Stable N-Heterocyclic Carbenes with a 1,1'-Ferrocenediyl Backbone and Their Heavier Homologues	**James Walton** *Durham University* A Study into Anticancer Pyridylphosphinate Metal Complexes	**Nilay Hazari** ★ *Yale University* Pincer Supported Iron Complexes for the Reversible Hydrogenation of CO_2 to Formic Acid and Methanol	**Simon Champet** *AMRSC* Graphene based materials for hydrogen storage
16.40-17.00	**Andrew Fensham-Smith** *University of Bristol* Gold(I) bipyridine complexes: Concise and efficient synthesis of electronically distinct cationic gold(I) complexes	**Stephen Mansell** *Heriot-Watt University* Synthesis and reactivity of fluorenyl-tethered N-heterocyclic stannylenes	**Isolda Romero-Canelon** *University of Warwick* Piano-stool complexes for cancer treatment: exploiting redox mechanisms	**Sam de Visser** *University of Manchester* Why are μ-nitrido bridged diiron(IV)-oxo porphyrins able to hydroxylate methane but mononuclear iron(IV)-oxo porphyrins not?	**John Lampkin** *University of Reading* Solvothermal Synthesis of Novel Oxothio Germanates

Wednesday 30th March 2016 (ctd.)

Plenary Lecture (L3) Session chair: Nick Le Brun

17.05 – 17.50 **Rachel Dunn**, *Durham* Chemistry and Education: Representation in the Teaching of John Dalton

18.00 – 19.00 Interest Group Committee meetings

19.00 – 19.30 Pre-dinner drinks

19.30 – 23.00 Conference Banquet (Panorama Suite, Rootes Building)

Thursday 31st March 2016

Plenary Lectures (L3) Session chair: Emma Raven

9.00 – 9.45 **Antoni Llobet**, *Institute of Chemical Research of Catalonia, ICIQ* Mechanisms Operating in Molecular Water Oxidation Catalysis

9.45 – 10.30 **Martin Warren**, *University of Kent* Modified Tetrapyrroles: Incarcerating a Goblin and a Devil

10.30 – 10.55 Tea/Coffee

Thursday 31st March 2016 (ctd.)

Parallel session 4

	Coordination & Organometallic	Coordination & Organometallic (2)	Main Group	Inorganic Biochemistry	Reaction Mechanisms	Publishing in Science
Room	L3	L5	L4	B202	B204/5	B201
Chair	Graeme Hogarth	Jon Rourke	Rebecca Melen	Dave Evans	Kylie Vincent	
10.55-11.15	**Michael Chapman** *University of Leeds* An Electrochemical Flow-Reactor for the Synthesis of Organometallic Complexes	**Sebastian Pike** *Imperial College London* In-situ identification of well-defined zinc cluster molecules during the synthesis of functional ZnO nanoparticles	**Maialen Espinal-Viguri** *University of Bath* Hydroboration of unsaturated C-C bonds using an iron complex	**Nicholas Barry** *University of Warwick* Combining Inorganic Medicinal Chemistry and Nanotechnology	**Abayomi Faponle** *University of Manchester* Reaction Mechanism of Cytochrome P450 Peroxygenase-Regioselectivity towards Biofuel Production	
11.15-11.35	**Philip Dyer** *Durham University* Highly selective ethylene trimerisation/tetramerisa-tion using PCN ligands	**Amanda Catherall** *University of Bath* Novel Precursors for the deposition of ZrO_2	**Steve Westcott** ★ *Mount Allison University* To B-E or not to B-E? Developing the Phosphinoboration Reaction	**Bethany Harriss** *Imperial College London* Functionalised Microbubbles for Dual-Modal Cancer Imaging	**Ruth Webster** *University of Bath* Exploring the rich chemistry of iron (II) ß-diketiminate complexes: from dehydrocoupling to hydrofunctionalisation	**Andrew Shore** *Editor,* *Dalton Transactions* Publishing Your Chemical Sciences Research
11.35-11.55	**Kevin Vincent** *University of Huddersfield* Proton-Coupled Mixed Valency in Hydrogen Bonded Dimers	**John Fielden** *University of East Anglia* Bis-Iminopyridine based Hydrogen Evolution Catalysts with Coordinating and Non-Coordinating Proton Relays	**Christine Thomas** ★ *Brandeis University* Chelating Ligands Incorporating Reactive N-Heterocyclic Phosphenium Cations	**Steve Archibald** *University of Hull* Copper(II) macrocyclic metal complexes for enhanced protein binding: biological activity and in vivo imaging	**Andrew Barker** *University College Dublin* Probing the Magnetic and Photophysical Properties of Manganese(III) and Iron(III) Spin Switches	
11.55-12.15	**Cinzia Imberti** *King's College London* New tris(hydroxypyridinone) chelators for 68Ga PET imaging	**Conrad Goodwin** *University of Manchester* Unprecedented f-Block Geometries Using Super-Bulky Ligands	**Robert Edkins** *University of Oxford* Tuning the Optical and Electronic Properties of Boron-Containing Electron-Acceptor Groups	**Jim Thomas** *University of Sheffield* Multifunctional Bioprobes	**Andrew Hones** *Durham University* Iridium Catalysed C-H Borylation of Indazoles	**Julia Weinstein** ★ *University of Sheffield* Ultrafast Photoinduced Charge Transfer in Metal Chromophores: towards directing photochemical pathways with bond-specific IR-excitation

Plenary lecture (L3) Session chair: Jon Rourke

12.20 – 13.05 **Peter Ford**, *University of California, Santa Barbara* Photo-Uncaging of Small Molecule Bioregulators from Metal Complexes

13.05 – 13.15 Closing remarks: David Cole-Hamilton (President) and Emma Raven (President-Elect)

13.15 Depart

Plenary Speakers at Dalton 2016

RSC Prize winners

Organometallic Chemistry Award 2015 Winner

Professor Todd Marder (Julius-Maximilians Universität Würzburg, Institut für Anorganische Chemie)
Fundamental studies of the synthesis, structure, bonding, reactivity and photophysical properties of organometallic compounds, and their applications in homogeneous catalysis and materials chemistry.

Homogeneous Catalysis Award 2015 Winner

Professor Pedro Pérez (Universidad de Huelva)
Development of alkane C-H functionalisation reactions, including those of methane, and other reactions catalysed by metal carbenes.

Creativity in Industry Prize 2015 Winner

Dr Christopher Barnard (formerly Johnson Matthey Technology Centre)

Research in the field of platinum group metal chemistry for catalytic and medicinal applications in industry.

Inorganic Mechanisms Award 2015 Winner

Professor Peter Ford (University of California, Santa Barbara)
Fundamental studies of mechanisms of inorganic photochemistry, homogeneous catalysis and the bioinorganic chemistry of nitric oxide and related nitrogen oxide species.

Interest Group Plenaries

Mike Lappert Memorial Lecture
Professor Eric Rivard (University of Alberta)
Fundamental synthetic inorganic chemistry with focus on the stabilisation of reactive intermediates/new bonding environments across the period table, and the generation of new polymeric materials for solar cell devices and active components for the electronics industry.

Professor Jonas Peters (California Institute of Technology)
Synthesis of novel first row transition metal complexes with relevance to living systems and energy materials, and studies of their electronic structures and reactivities.

Professor Martha Greenblatt (Rutgers)
Synthesis and crystal growth of novel transition metal compounds with quasi-low-dimensional properties, including perovskite-related manganates, coboltates and ferrates, transition metal oxide bronzes, metal cluster chalcogenides, transition metal nitrides, and high temperature superconductors.

Professor Claire Carmalt (University College London)
Application of organometallic chemistry to problems in materials deposition, most notably the development of "designed" molecular precursors targeted for thin film growth by chemical vapour deposition (CVD).

Professor Antoni Llobet (Institute of Chemical Research of Catalonia, ICIQ)
Mechanistic studies of redox catalysis by transition metal complexes for technological applications, including catalytic oxidation of water to dioxygen (artificial photosynthesis) and photo-production of hydrogen from water and sunlight.

Professor Martin Warren (University of Kent)
Biosynthesis and biology of the pigments of life, encompassing metallocofactor molecules such as vitamin B12, heme and siroheme, and synthetic biology approaches to reconstructing whole synthetic pathways in cells.

Special Plenary to mark the 250th anniversary of the birth of John Dalton

Rachel Dunn (University of Durham)
Representation in nineteenth-century chemistry through the life and career of John Dalton.

Sir Geoffrey Wilkinson Dalton Poster Competition

The Geoffrey Wilkinson Foundation will sponsor the annual Dalton Poster competition at Dalton 2016.

The poster competition is divided into two parts: one for postgraduates, and one for postdoctoral researchers. The winner of each section will receive a £1000 bursary to attend an international conference of their choice, and there will also be runner-up prizes of £100 each.