Imperial College London is a world leading university. In 2011 the *Times Higher Education* placed us 3rd in Europe and 8th in their World University Rankings. As the central science chemistry has been a major contributor to this success. We were also ranked 11th in the QS World University subject rankings.

The Department of Chemistry is at the forefront of modern Chemistry research, both in our core discipline and at the interfaces of chemistry with other subjects. We collaborate widely across the College, the UK and the world. We are committed to both fundamental science and applications orientated research, seeing these as a common endeavour. We are very proud of our many collaborations with industry. We are an international centre of excellence for chemistry; the 2008 RAE showed that our senior academics are all recognised leaders in their fields and that they are joined by a fantastic group of rising stars, who will be the leaders of tomorrow. In 2012 we won five internationally recognised scientific awards and Sue Gibson was awarded an OBE for services to science. We don’t forget the importance of teaching either, and four of our academics were given teaching awards and four of our support staff were given awards for supporting teaching from the Rector. On top of all of this, in the College’s 2011 staff survey, chemistry came out as one of the happiest departments in which to work. This is made possible by the superb academics, support staff, researchers and students in the Department, who do all of the hard work, and contribute to making us the vibrant, diverse community that we are.

This review gives a snapshot of some of our research activities in 2012. I hope that it conveys to you some of the excitement of the research of Imperial’s Department of Chemistry. For more information please go to our website at www.imperial.ac.uk/chemistry.

Best wishes

Tom Welton
The Department of Chemistry continued to thrive and develop in 2012 with a range of successes including major grant awards and fellowships and recognition for the great scope and depth of our research activities. Some of our Department's highlights of the year have been identified below.

Honours and awards
The research of the Department's academics continues to be recognised with a series of prestigious awards including:

Professor Sue Gibson who received an OBE for her services to chemistry and science education in the New Year Honours List.

Professor Andrew Holmes awarded a Royal Society Royal Medal for his contribution to the science of organic plastic electronics. The Royal Medal is one of the Society's premier awards issued to three top scientists a year. Former recipients include Charles Darwin and Francis Crick.

Professor James Durrant awarded the RSC Tilden Prize for his world-leading contributions to the function and design of molecular and nanostructured materials for solar energy conversion.

Professor Tony Cass honoured with a RSC National Chemical Landmark Plaque for his work on the creation of a sensor allowing diabetics to easily and accurately monitor their blood sugar.

Dr Ed Tate won the 2012 Wain award, a prize given to an outstanding young scientist in the Biochemistry area. The prize consists of a silver medal, £1,000 in prize money and a lecture which was delivered by Dr Tate at the University of Kent in October 2012 and entitled Using chemistry to target protein modification in disease.

Dr Marina Kuimova a rising star in the Department received both the British Biophysical Society's Young Investigator's Award for 2012 and also the RSC Harrison Meldola Prize for her pioneering studies in the spectroscopy and imaging of biological materials, as exemplified by her development and application of fluorescent molecular rotomers to measure cellular viscosity.

Professor Lord Porter of Luddenham a decade after his death, the Noble Prize winner, who revolutionised the study of chemical kinetics was honoured by the Royal Society of Chemistry with a commemorative National Chemical Landmark blue plaque at the Department of Chemistry.

Dr Joshua Edel elected to the Court of Imperial College London.

Professor Tom Welton and Drs Chris Braddock and James Wilton-Ely all received 2012 President & Rector’s Awards for Excellence in Teaching and Professor Alan Spivey received the Rector’s medal for his Outstanding Contribution to Teaching Excellence.

Other awards were given to the following chemistry staff in recognition of their contribution to learning and teaching within the Faculty of Natural Sciences: Rajdeep Sandhu, Chris Howard, Deejay Kistnah and Jack Paget all received Faculty of Natural Science Awards for their Support of Excellence in Teaching.

FELLOWSHIPS
The following staff members were awarded fellowships in 2012:

Drs Andrew Ashley and Chris Cordier were awarded Royal Society University Research Fellowships.

Drs Jorge Bures Amat, Kevin Lovelock and Hugo Bronstein were awarded Imperial College Junior Research Fellowships.

Dr Ling Ge awarded a British Science Association Media Fellowship which she undertook at the Financial Times.

Drs Mark Rackham and Megan Wright were awarded EPSRC Doctoral Prize Fellowships which are reserved for the very best newly qualified PhDs who received EPSRC studentship funding.

The Department was also awarded seven Marie Curie Fellowships.

Research portfolio
The Department of Chemistry has a thriving research portfolio with research volume totalling £13.3 million in 2011–12. The breakdown of research funding for 2011–12 is detailed below:

Research Councils accounted for 55% of the Departments research funding and is testament to our continued success in leveraging funds from the RCUK, and in particular, the EPSRC.

Europe accounted for 14% of the Department’s research funding. This has been a result of strategic initiatives within the Department to engage with Europe and we have been rewarded with substantial success in ERC and Marie Curie Fellowship schemes.

Industry accounted for 17% of the Department’s research funding. The Department continues to work collaboratively with new and traditional industrial funders. Significant industrial funders in the Department include INEOS, Rio-Tinto, GSK and BP.

Charity accounted for 11% of the Department’s research funding. Significant charity funders include the Wellcome Trust, the Leverhulme Trust and Cancer Research UK.

Government accounted for 3% of the Department’s research funding.

Publications
Publication successes included:

- Professor Robin Leatherbarrow and Dr Ed Tate’s article: Chemical and biomimetic total syntheses of natural and engineered MCoTI cyclotides was one of the 10 most highly cited articles in the area of natural products, in OBC since it started 10 years ago.
• Dr Tim Albrecht and his collaborators won the award for the Best Paper at the IEEE International Conference on Electronics, Circuits, and Systems (ICECS) 2012.

• Professors Charlotte Williams and Richard Templer, Drs George Britovsek and Jason Hallett’s (plus collaborators) paper: The path forward for biofuels and biomaterials exceeded 1,000 citations.

• Professor Alexei Kornyshev and his research group’s paper: Chiral electrostatics breaks the mirror symmetry of DNA supercoiling, was selected for inclusion in the Institute of Physics select publication list IOP Select which includes articles selected for their quality and recency.

• Dr Andrew Ashley’s first paper from Imperial was one of the top 10 (7th) accessed in Dalton Transactions for April 2012.

Outreach activities
The Department has a member of staff within the Outreach Office who organises and runs a large variety of events to promote the Department to prospective students.

In 2012, the Department was involved with three different summer schools with students aged 15–17. These included two weeks of the popular STEM World Summer School where students aged 15–17 undertook an advanced chemistry course working on synthetic chemistry experiments designed for undergraduates, and one week of the new Sutton Trust Summer School. This course saw students aged 16–17 undertake short research projects including investigations into how the size of silver nanoparticles are influenced by their synthetic variables and investigations into different amines that can be used in carbon capture reactions.

In addition to the summer schools, there were a large number of day events organised for school aged students. The annual department taster days, designed for year 12 students, saw around 120 prospective students attend the Department over two days in June, with both available dates being fully booked before the beginning of April. The Department also hosted the annual Salters’ Festival for year seven and eight students which has now been running for seven years; a number of A-level masterclasses and spectroscopy workshops designed to enhance the spectroscopy teaching for year 12 and year 13 students, and the RSC Top of the Bench Final which saw students from across the UK competing in the final of this national competition. In addition, the Department also hosted chemistry masterclasses for students in year 11 and year 12 during the Easter break. These workshops were funded by the College’s Access Fund for students who are considered to be from a widening participation background but gave the students a taste of what it is like to work within an undergraduate laboratory.

Finally, as a new addition to the programme, January 2012 saw the start of the Department being involved with the Royal Society of Chemistry’s Spectroscopy in a Suitcase initiative. The RSC have provided a portable IR spectrometer and a UV spectrometer with funding to enable this kit to be taken to schools by chemistry ambassadors. This has proved to be extremely popular and we trained circa 20 ambassadors in December 2012 to keep up with the increased demand.

Overall in 2012, it is estimated that approximately 760 students benefited from the activities run either by the Department or in conjunction with the Department. Many undergraduate and postgraduate students were involved in these activities, working with the participants as mentors, in addition to the technicians and academic staff who support the activities with their time.

Promotions and appointments
Professor Phil Parsons formerly of the University of Sussex joined the Department as Senior Research Investigator and Professor Keith Willison joined the Institute of Chemical Biology as Chair of Chemical Biology.

In July 2012 Visiting Professor Vernon Gibson was appointed as Scientific Advisor to the Ministry of Defence.

Dr Tim Albrecht appointed as Director of Postgraduate Studies.

Staff promoted in 2012:
To Professor
Charlotte Williams and Sophia Yaliraki
To Reader
Martin Heeney and Ed Tate
To Senior Lecturer
Matt Fuchter

NEW APPOINTMENTS IN 2012
Dr Kevin Lovelock
Junior Research Fellow
Kevin completed his MSci at the University of Nottingham (2000–04) and PhD in Ultra-High Vacuum Surface Science, focussing in particular on ionic liquids, under the supervision of Professor Rob Jones (2004–08). He subsequently held postdoctoral positions at Erlangen-Nuernberg University under the supervision of Professor Hans-Peter Steinrück, University of Nottingham under the joint supervision of Dr Darren Walsh and Dr Peter Licence, and University College London under the supervision of Dr Susan Perkin. His postdoctoral projects included investigating the surface science, vaporisation, electrochemistry and confinement of ionic liquids. In 2012 Kevin was awarded an Imperial Junior Research Fellowship. His current work focuses on understanding and predicting ionic liquid properties, primarily through investigating the bulk and surface energetics of these fascinating materials. These studies underpin a number of key applications of ionic liquids, including their use as solvents for self-assembly and as electrolytes in supercapacitors.

Professor Keith Willison
Professor in Chemical Biology
Keith obtained his PhD from the MRC Laboratory of Molecular Biology in Cambridge working with the first sets of monoclonal antibodies to discover new developmental and tumour markers (1975–78) and then moved to Cold Spring Harbor Laboratory, USA to learn how to clone genes (1979–81). He was appointed group leader at the Institute of Cancer Research (ICR) in London helping to introduce recombinant DNA technologies to the study of cancer processes. He has worked on protein folding mechanisms and molecular chaperones for 20 years and has discovered a unique energy folding landscape for the ubiquitous protein, actin, which forms muscles.
and shapes our cells. He was Head of Laboratories at the ICR (1995–2005) helping to treble the size of the Institute and rebuild and reorganise it on two sites across London.

He is a founder member of the Chemical Biology Centre, working with colleagues in the Department of Chemistry since 2002. He left the ICR in 2011 and was Weston Visiting Professor in the Department of Structural Biology at the Weizmann Institute of Science, Israel before joining Imperial in the spring of 2012. He is co-holder of the Chemical Biology Doctoral Training Centre, Single Cell Proteomics and Proxomics grants and a member of the Executive of the Institute of Chemical Biology. Presently he is working on single molecule approaches to protein folding mechanisms and protein counting in single cells.

The Charles Rees Prize Fund

In 2008 the Department of Chemistry chose to honour the memory of Professor Sir Charles Rees with the launch of a fund to award scholarships to the very best chemistry students to support their PhD studies at Imperial. The fund continues to grow due to generous support from alumni and industrial partners. If you wish to contribute to this fund you can do so by completing the form at the back of this review, or via our website:

www.imperial.ac.uk/chemistry
Research in the catalysis and advanced materials section is directed towards the design, synthesis and utilisation of new catalyst systems, an understanding of their mechanism of action – particularly in ionic liquids, and the synthesis and application of functional compounds and materials within industry, medicine and society.

Key areas of interest include (i) the development of environmentally sustainable (‘green’) technologies (metal and non-metal catalysts, solvents and processes i.e. carbon management), (ii) pioneering rigorous mathematical and kinetic analysis of complex organic reactions and reaction networks and (iii) design and evaluation of multi-modal imaging probes for biomedical imaging. Fundamental scientific advances have been illustrated in each area, alongside strategic and exciting applications within the chemical and pharmaceutical industries.

**Current activities in catalysis include:**
- Homogeneous catalysts for carbon management
- Reaction kinetics of catalytic reactions and processes
- C-C and C-N coupling reactions
- Metallocene and non-metallocene polymerisation technology
- Olefin metathesis and metathesis polymerisation
- Sustainable chemistry
- Low temperature Fischer-Tropsch catalysis
- Redox-active and hemilabile ligands
- Privileged and chiral ligands
- Systems chemistry
- Ligand design (organometallic chemistry)
- Oxidation catalysis
- Asymmetric and enantioselective synthesis

**Current activities in materials include:**
- Using solvent effects and environmentally friendly solvents
- Fast and targeted synthesis for medical imaging
- Biodegradable materials
- Biosustainable polymers
- Electroluminescent metal-containing materials
- Organometallic polymers
- Polyoolefins
- Polylactides
- Chiral ligands
- Biomedical imaging probes
- Microreactors and microfluidics
- Ionic liquids
The research undertaken in the CB section broadly uses tools and insights derived from the physical sciences to probe, analyse and manipulate the complicated systems of biology. It focuses on experimental and theoretical topics relevant to the understanding of biological macromolecules and biological systems in terms of the principles and methods of physics, chemistry and mathematics, bringing quantitative molecular sciences into the biological arena.

The CB section conducts research concerned with understanding the interplay between various systems within cells, including the interactions between DNA, RNA and protein biosynthesis, as well as how these events are regulated. By drawing knowledge and experimental techniques from a wide variety of disciplines, they are able to directly observe, model or even manipulate the structures and interactions of individual molecules or complexes of molecules. They investigate the ongoing integration of chemical and systems biology and the essential role of chemical biology in drug discovery and development. More specifically they study the use of natural products and their analogs, strategies for small-molecule control of protein function and properties, methods for predicting which molecules will display desirable biological properties, the synthesis of bioactive molecules and the newly developing area of chemical genetics. They target protein families, cellular and organismal delivery of molecules, and the use of systems biology to model cellular responses to small molecule–induced perturbations.

There is a close relationship between chemical biology practices in academia and drug development methods in the pharmaceutical industry: technologies such as high-throughput screening, chemical informatics and mathematical modelling of cellular pathways are the basic tools of both. Many links can be found between researchers in the CB section and industry, involving and integrating their chemical biology research within the wider framework of research and development related to drug discovery.

Dr Laura Barter, Dr Nicholas Brooks, Professor Tony Cass, Dr Oscar Ces, Dr Ian Gould, Professor David Klug, Dr Rob Law, Professor Robin Leatherbarrow (Head of Section), Dr Joachim Steinke, Dr Ed Tate, Professor Richard Templer, Professor Ramon Vilar, Professor Keith Willison, Dr Rudiger Woscholski and Professor Sophia Yaliraki
One major research activity within the Section involves experimental, simulation and/or theoretical studies across a wide range of topics spanning modern analytical science (nanofluidic devices for bioanalytical applications; electrochemical sensors), electrochemistry (solvation and ionic liquids; semiconductors; redox-mediated conductance through single molecules), energy research (energy transfer across nanoscale interfaces; fuel cells; catalysts; batteries; hydrogen storage; supercapacitors), interfacial chemical physics (electrowetting and electrovariable optics; wetting at fluid interfaces; nanofluidics), soft matter and biophysical chemistry (self-assembled monolayers and bilayers; DNA interactions; aggregation and recognition; liquid crystals and model membranes; lipid microbubbles for ultrasound imaging), and optical imaging (fluorescence imaging microscopy of cells and photodynamic therapy).

A second major activity lies in computer-based modelling of chemical systems. The quantum chemistry group studies a broad range of topics in computational chemistry, such as non-adiabatic reactivity, large scale density functional simulations, and photochemistry. The group is internationally recognised for the development of the widely used GAUSSIAN package, and runs the EPSRC NSCCS (National Service for Computational Chemistry Software). Outreach is championed by Emeritus Professor David Phillips CBE, who gives a large number of public chemistry lectures each year.

Dr Tim Albrecht, Dr Mike Bearpark, Dr Fernando Bresme, Dr Joshua Edel, Dr Patricia Hunt, Professor Alexei Kornyshev, Professor Anthony Kucernak, Dr Marina Kuimova, Dr Kevin Lovelock, Professor David Phillips CBE (Emeritus), Professor Nick Quirke, Professor Mike Robb, Professor John Seddon (Head of Section) and Dr Paul Wilde
The Nanostructured Materials and Devices section specialises in the synthesis, characterisation and exploitation of semiconductor and nanostructured materials for novel applications in optoelectronics, photonics, nanotechnology and chemical/biological analysis. Their research interests involve harnessing a wide variety of materials, including inorganic semiconductors, organic semiconductors, nanoparticles and nanotubes. Strong emphasis is placed on exploiting the unique properties of nanostructured materials and their implications for nanoscale science. All members of the section play an active role in the London Centre for Nanotechnology (LCN), a joint research centre recently established between Imperial College London and University College London.

Major current research activities include:

- Atomically controlled growth and characterisation of semiconductor nanostructures
- Organic semiconductors and their application in light emitting diodes and photodetectors
- Development of low cost organic solar cells
- Controlling interfacial properties in organic electronics
- Synthesis and characterisation of carbon and inorganic nanotubes
- Synthesis and characterisation of metal and semiconductor nanoparticles
- Surface modification of nanotubes for composites and electrodes
- Microfluidics and Nanofluidics
The Synthesis Section research programme is focused on the synthesis, characterisation and application of novel organic, organometallic, inorganic and metal organic compounds. Current projects include the total synthesis of bioactive natural products such as antibiotics, antifungal agents, antiviral compounds and anticancer agents. These endeavours, which include the design of new synthetic methodology, enantioselective transformations, heterocyclic chemistry, parallel synthesis and combinatorial chemistry, are directly relevant to pharmaceutical and agrochemical innovation. Research also includes the development of sustainable synthetic chemistry including catalytic enantioselective and atom economic syntheses. The synthesis and computational studies of dendrimers, speciality polymers, including conjugated polyaromatics, heterocyclic block copolymers, ring opening metathesis polymers and modified lactides, are being prepared for parallel synthesis, as non-linear optical materials, for molecular recognition, and as organic semiconductors in electronic applications.

Research on main group and organometallic synthetic chemistry is directed towards organosilicon compounds including novel bridged main group element cations and silsesquioxanes, improved copper-based catalysts for modified-Ullmann coupling, studies on the reactivity and structures of s-block organometallics and related heterobimetallic species, and alkene and alkyne metathesis reactions. Bespoke Metal Organic Framework (MOF) materials are currently under development with applications in hydrogen storage, carbon dioxide capture, magnetocaloric cooling and heterogeneous catalysis. Communication between the metal centres of multimetal complexes and its impact on photophysics with the ultimate goal of ‘molecular electronic’ applications is under investigation.

Current activities include:
- Green and sustainable synthetic organic chemistry and catalysis
- The synthesis of heterocyclic compounds
- The total synthesis of biologically active natural products
- Parallel synthesis and combinatorial chemistry
- Medicinal chemistry with focus on cancer and cardiovascular disease
- Speciality polymer synthesis
- Organometallic and main group chemistry
- The use of siloxanes as novel solvents
- Silsesquioxanes as precursors to novel materials
- Synthesis of metal-organic framework materials for hydrogen storage and carbon capture technologies
- Using solvent effects in synthesis
- Physical organic chemistry

Professor Alan Armstrong, Professor Anthony Barrett (Head of Section), Dr Chris Braddock, Dr James Bull, Professor Donald Craig, Dr Rob Davies, Dr Matthew Fuchter, Professor Sue Gibson, Professor Andrew Holmes, Dr Paul Lickiss, Professor Henry Rzepa and Professor Alan Spivey
The research interests of Dr Tim Albrecht and his group span a range of different areas from single-molecule conductance studies in molecular electronics to organocatalysis, especially organocatalysis and enantioselective catalysis. His group applies these skills to the determination of in situ reaction monitoring, kinetics and computational modelling. They are also active at the interface with biology, including protein-ligand engineering, synthesis of molecular affinity- and activity-based probes, and new methods for drug discovery.

**2012 Publications**

- Albrecht T. *Electrochemical tunnelling sensors and their potential applications*. Nature Communications, 01/05/2012, 3, 829.

**Professor Alan Armstrong (Synthesis)**

Synthetic organic chemistry; asymmetric synthesis; catalysis; mechanism; chemical biology; synthesis of bioactive compounds. Professor Alan Armstrong’s core expertise is in synthetic organic chemistry: this includes catalysis, especially organocatalysis and enantioselective catalysis. His group applies these skills to the determination of catalytic reaction mechanisms using in situ reaction monitoring, kinetics and computational modelling. They are also active at the interface with biology, including protein-ligand engineering, synthesis of molecular affinity- and activity-based probes, and new methods for drug discovery.

**ORGANOCATALYSIS**

Professor Armstrong and his group are involved in the development of small organic molecules as catalysts, an area known as organocatalysis. Organocatalytic reactions have the advantage that they can usually be carried out without rigorous exclusion of air or water, and they avoid the use of potentially toxic transition metal reagents. Following on from early work in the development of new organocatalysts for alkene epoxidation, the group are currently focusing on asymmetric synthesis involving nitrogen transfer. They have developed a novel, efficient and highly stereoselective amination/sigmatropic rearrangement of allylic sulfides which provides access to vinyl glycine derivatives, and are exploring further applications of this concept. Aziridines are highly useful synthetic building blocks and the group have developed a novel amine-catalysed alkene aziridination procedure, proceeding via aminimine intermediates. Synthetic applications of this chemistry are currently being exploited.

In collaboration with Professor Donna Blackmond (Scripps), the Armstrong group are elucidating the mechanisms of key organocatalytic reactions using synthesis, kinetics, spectroscopy and computation. In particular, studies of the effects of additives in aminocatalysed alpha-functionalisations of carbonyl compounds have revealed a remarkable reversal of product enantioselectivity. In another mechanistic study, in collaboration with Dr Chris Braddock, we are elucidating the mechanisms of cinchona alkaloid-catalysed enantioselective bromocyclisations, with additives again being found to exert marked effects on enantioselectivity.

**CHEMICAL BIOLOGY**

In collaboration with Dr D Mann (Biological Sciences), the Armstrong group are engaged in the development of new molecular probes to allow improved understanding of protein phosphorylation/dephosphorylation mediated by cell-cycle kinases and phosphatases. This includes a novel combination of protein-ligand engineering and affinity labelling to allow identification of the protein substrates of specific kinases. We are developing activity-based probes to profile phosphatase activity alongside a programme aimed at developing small molecule inhibitors of cdc25, a phosphatase implicated in cancer. We are developing a new approach, ‘kinetic template-guided tethering’, aimed at discovery of inhibitors of protein-protein interactions. Finally, in a Royal Society Industry Fellowship, Professor Armstrong is working with Pfizer Neusentis to develop chemical biology tools to allow improved understanding of the function of ion channels which are targets for pain therapy.

**2012 Publications**

of such a transformation are the recently discovered ‘Frustrated Lewis Pairs’ (FLPs) which are based on non-metal components such as amines and Lewis acidic boranes. In conjunction with efforts to design new thermally and hydrolytically stable FLPs, novel metal-based systems capable of effecting the reversible splitting of hydrogen are also being investigated. The primary goal is then to effect the hydrogenation of important small molecules (which are coordinated to transition metal based co-catalysts), mediated by sequential ‘proton coupled hydride transfer’ using activated hydrogen. Since hydrogen can be synthesised from the splitting of water using renewable solar energy we can obtain routes to the chemical storage of hydrogen and thus energy.

**UTILISATION OF THESE STRATEGIES ENABLES THE DESIGN OF MULTI-COMPONENT SYSTEMS TO SUSTAINABLY EFFECT THE:**

**Hydrogenation of carbon dioxide or carbon monoxide into hydrocarbons and water**

In the case of carbon monoxide this is known as the Fischer-Tropsch (FT) process and is currently performed heterogeneously and at elevated temperatures and pressures; it generally exhibits poor selectivity. Since carbon monoxide can be made through the hydrogenation of carbon dioxide (albeit endothermically), conducting this reaction in parallel with a homogeneous FT reaction (strongly exothermic) would enable the conversion of carbon dioxide and hydrogen into energy-dense liquid hydrocarbons for use as carbon-neutral ‘green’ fuels, or feedstock chemicals (carbon sequestration). Such co-catalysts are based on mid-late transition metals of the 1st and 2nd row.

**Fixation of dinitrogen to ammonia**

The Haber process produces all synthetic ammonia from dihydrogen and dinitrogen that humans use for fertiliser to improve agricultural yields and hence feed the world population. However, it does so at an immense energy cost (ca. 2% global energy demand) due to operation at high temperatures and pressure. Since iron is used as a catalyst in the heterogeneous reaction, co-catalytic dinitrogen iron(II) complexes as reducible substrates. Systems capable around the catalytic activation of dihydrogen into proton and hydride equivalents, in order to bring about a step change in the reactivity of the hydrogen molecule with reducible substrates. Systems capable

**2012 Publications**

Herrington TJ, Thom AJ, White AJ, Ashley AE

*Novel H₂ activation by a tris[3,5-bis(trifluoromethyl)phenyl]borane frustrated Lewis pair*  
*Dalton Transactions, 25/04/2012, 41, 9019–9022*

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**Professor Anthony G M Barrett (Synthesis)**

Professor Tony Barrett has carried out extensive research on the synthesis of bioactive natural products and the underlying synthetic methodology. Recently, his group has been very active in the total synthesis of quinone, resorcylate and terpene-resorcylate natural products including angelicon A, hericenone J and hericenol A and cruentarin A. Methodology that has been developed includes tunable dioxine thermolysis, transanular macrocyclisation and aromatisation to produce complex resorcylates and multi-component benzyne coupling reactions.

Professor Barrett has designed new catalysts for important chemical transformations. These include the use of recyclable, water tolerant lanthanide and bismuth triflates and triflides for electrophilic arene nitrotations and Friedel Crafts reactions, in esterifications, in the conversion of penicillins to cephalosporins and for benzylic oxidations to provide ketones and arene carboxylic acids. He has applied alkene metathesis in natural product and medicinal chemistry areas including macrocyclic peptidomimetics, viridiofungins, clavilactone B and apicidan analogues. Finally, in collaboration with Dr Mike Hill, he has applied alkaline earth catalysts for hydroamination, hydrophosphination and other important reactions.

The Barrett group in collaboration with B.M. Hoffman at Northwestern University have synthesised new classes of porphyrines and secoporphyrines. These show unusual coordination chemistry and are of considerable use as novel magnetic and optical materials, as imaging agents for the early stage detection of cancer and in photodynamic therapy. Porphyrines with peripheral thiol, alcohol or amine groups are able to complex metal ions to the edges of the macrocycle in addition to the binding within the central cavity and form multimetallic complexes. Such peripheral metal binding is important in the development of new sensors as well as supramolecular arrays. Finally, in collaboration with Professor R Charles Coombes and others in Cancer Medicine at Imperial and Professor Dennis Liotta at Emory University, the Barrett group has major programmes in the computer-assisted design, synthesis and biological evaluation of small molecule inhibitors of key enzymes involved in cancer including highly selective CDK7 inhibitors and inhibitors of other cancer relevant targets.

**2012 Publications**

Laclef S, Anderson K, White AJP, Barrett AGM

*Total synthesis of amorfrutin A via a palladium-catalyzed migratory prenylation-aromatization sequence*  

Brinkmann C, Barrett AGM, Hill MS, Procopiou PA

*Heavier alkaline earth catalysts for the intermolecular hydroamination of vinylarenes, dienes, and alkynes*  
*Journal of the American Chemical Society, 18/01/2012, 134, 2193–2207*

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**Dr Andrew Ashley (CAM)**

Dr Andrew Ashley’s research interests pivot around the catalytic activation of dihydrogen into proton and hydride equivalents, in order to bring about a step change in the reactivity of the hydrogen molecule with reducible substrates. Systems capable...
and computational modelling to reveal pathways, mechanisms and rate limiting steps that control the light dependent and dark Photosynthetic reactions.

For example, members of her group are studying a network of enzymes, which create organic carbon from the CO₂ in the air but are strikingly inefficient. Typical enzymes can process ~1000 molecules per sec, but one of the enzymes, Rubisco, involved in the network, fixes only about three CO₂ molecules per sec. Barter is particularly interested in the regulatory mechanisms dictating Rubisco’s inefficiency. Collaborators include Dr Rudiger Woscholski, Professor Mauricio Barahona, Dr Sophia Yaliiraki, Dr Ian Gould and Dr James Murray.

A collaboration with Dr Ian Gould, and Dr Rudiger Woscholski is developing a novel, generic chaperon assay to probe protein-protein AAA+ interactions. This project is currently investigating the interaction between Rubisco and Rubisco activase (a AAA+ protein).

Dr Barter is also interested in developing novel chemical biology tools, based on Carbonic Anhydrase Mimics, aimed at enhancing photosynthetic carbon fixation. This project is in collaboration with Professor Nicholas Long and Dr Rudiger Woscholski. The novel compounds are being tested with respect to their specificity and affinity, by the Barter group, using Rubisco based assays.

In collaboration with Dr Thorsten Hamann her group is investigating the relationship between cell wall biosynthesis and Rubisco and Rubisco Activase activity. Previous work has shown that photosynthetic activity is partially regulated by carbohydrate sinks. However, this coordination is not well understood.

Barter is a member of a collaborative team working on research funded by the EPSRC Cross-Disciplinary Feasibility Account entitled ‘Elements of a Vesicle Machine’: This is with Dr Oscar Ces, Professor RichardTempler, Dr Rob Law, Professor John Seddon, and Professor Paula Booth, (Bristol). One theme of this research recently demonstrated a novel form of protein communication, which employs harnessed mechanical energy within the biological membrane to promote controlled communication between proteins.

Dr Barter is Co-Deputy Director of Institute of Chemical Biology Centre for Doctoral Training, which successfully passed its mid-term review in 2011. She is a member of the Institute of Chemical Biology’s Research and Operations Board.

Dr Barter is Co-Director with Dr Rudiger Woscholski of AGRI-net (www.agri-net.net), a EPSRC and BBSRC funded agri-science chemical biology network focused on developing novel tools and technologies aimed at alleviating bottlenecks in the agri-sciences. This network has Professor Stuart Dunbar (Syngenta) and Dr Angela Karp ( Rothamsted Research Institute) on the executive board.
Dr Michael Bearpark (CP)

The Computational Photochemistry group studies the photostability, photochemical reactivity, and radiationless decay of molecules of all sizes.

In collaboration with Gaussian Inc. (www.gaussian.com), the ONIOM computational method has been extended to study electronic excitation and deactivation processes taking place in biological chromophores. For the photoreceptor protein rhodopsin, for example, our calculations showed that introduction of a second charged residue (deprotonation of Glu181) into the retinal-binding pocket leads to remarkably small differences in key properties, particularly the $S_1>S_0$ and $S_2>S_1$ vertical excitation energies, challenging the accepted view. The geometry changes in molecular excited states that promote ultrafast internal conversion can also now be studied with ONIOM. This work forms the basis of a joint EPSRC/NSF award to a collaboration with the experimental groups of Jasper Van Thor (Molecular Biosciences, Imperial) and Paul Champion (Northeastern University, Boston).

Earlier calculations by the group showed how the shape and accessibility of crossings of potential energy surfaces determines the outcome of a photochemical reaction. ‘Sloped’ crossings in particular can promote ultrafast radiationless decay, coherent oscillations, and also photostability – decay back to reactants – in molecules ranging from pesticides and dyes to polycyclic aromatic hydrocarbons (PAHs) found in the interstellar medium, such as perylene radical cation. (The astrochemistry component of this work is now carried out as part of the French ANR-funded consortium GASPARIM: Gas-phase PAH research for the interstellar medium). Algorithm and code developments carried out in the group remain central to these investigations, suggesting ways of engineering molecules to be photostable.

State crossings are also crucial for the successful operation of photochromic molecules and photoswitches, which depend on whether two isomers of a molecule can be successfully interconverted by absorbing light of different wavelengths. For example, dihydronaphthalene is not photochromic because of multiple reaction pathways leading to and from the excited state decay funnel, but fulgides are in general, as these pathways have effectively been eliminated.

Calculations modelling excited state decay explain why DHN is not a good photoswitch

2012 Publications


Serrano-Pérez JJ, Bearpark MJ, Robb MA The extended $S_1/S_0$ conical intersection seam for the photochemical 2+2 cycloaddition of two ethylene molecules Molecular Physics, 27/06/2012, 110, 2493–2501


Dr Chris Braddock (Synthesis)

The Braddock Group is engaged in stereoselective synthesis, organo- and transition metal catalysis, and natural product synthesis. In particular, we have recently developed the first methodology for the generation of enantiomerically pure bromonium ions, and continue to explore and exploit biomimetic electrophilic bromination for the synthesis of complex halogenated natural products.

In our continued efforts to synthesise naturally occurring halogenated marine metabolites by biomimetic methods, we have published a full article in the Journal of Organic Chemistry detailing a unifying stereochemical analysis for the formation of halogenated medium-ring ethers in marine red algae from a single biogenetic precursor. These compounds have long inspired the worldwide development of synthetic methodology for the formation of medium rings, but each of their diverse structures have required bespoke synthetic solutions. Our unifying analysis can account for ring-size, the position of the halogen substituents, and relative and absolute configurations of all the known natural products. We have now experimentally corroborated the feasibility of this process for concurrent formation of 7-, 8- and 9-ring ethers corresponding to the halogenated medium-ring ethers of known metabolites using a model compound.

We have also reported in Chemical Communications the first example of a dyotropic rearrangement of an enantiomerically pure, conformationally unconstrained, vicinal dibromide. This has solved a long-standing problem in the area.
2012 Publications
Bonney KJ, Braddock DC
A unifying stereochemical analysis for the formation of halogenated Cn-
acetonitrile medium-ring ethers from Laurencia species via intramolecular bromonium ion assisted epoxide ring-opening and experimental corroboration with a model epoxide
Braddock DC, Roy D, Lenoir D, Moore E, Rzepa HS, Wu JI, Schleyer PV
Verification of stereospecific dyotropic racemisation of enantiopure D and L-1,2-dibromo-1,2-diphenylethane in non-polar media
Chemical Communications, 2012, 48, 8943–8945

Dr Fernando Bresme (CP)

Our research is concerned with the investigation of the structure and dynamics of complex interfaces of chemical relevance: colloids, biopolymers, membranes and nanomaterials. The interfacial physico-chemical behaviour often confers striking properties to these materials, by mediating and promoting a whole range of chemical processes. One of our main areas of interest is the investigation of energy transport through nanoscale interfaces. Current efforts are directed towards the development of computational tools to quantify thermal transport across these interfaces, and the application of these tools to design high performance materials for energy management problems (e.g. super-insulating and highly conductive media) and nanomaterials with chemical and medical applications (e.g. catalysis, medical therapies).

We are particularly interested in the investigation of novel physical concepts for energy conversion and energy recovery applications (e.g. recovery of waste heat). We combine non-equilibrium and equilibrium computer simulations, non-equilibrium thermodynamics theory and experiments to investigate energy conversion processes in molecular machines.

2012 Publications
Römer F, Bresme F
Heat conduction and thermo-molecular orientation in diatomic fluids: a non equilibrium molecular dynamics study
Molecular Simulation, 01/06/2012, 38, 1198–1208
Römer F, Bresme F, Muscatello J, Bedeaux D, Rubi JM
Thermo-molecular Orientation of Nonpolar Fluids
Physical Review Letters, 01/03/2012, 108, 105901 – 105901
Tarazona P, Chacon E, Bresme F
Intrinsic profiles and the structure of liquid surfaces
Journal of Physics-Condensed Matter, 18/07/2012, 24, 284123
Lervik A, Bresme F, Kjelstrup S
Molecular dynamics simulations of the Ca2+-pump: a structural analysis
Physical Chemistry Chemical Physics, 01/01/2012, 14, 3543–3553
Lervik A, Bresme F, Kjelstrup S, Rubi JM
On the thermodynamic efficiency of Ca2+-ATPase molecular machines
Biophysical Journal, 19/09/2012, 103, 1218–1226
Tarazona P, Martinez H, Chacon E, Bresme F
Newton black films as wetting systems
Physical Review B, 02/02/2012, 85, 085402
Bresme F, Chacón E, Tarazona P, Wynveen A
The structure of ionic aqueous solutions at interfaces: an intrinsic structure analysis
Journal of Chemical Physics, 21/09/2012, 137, 114706

Römer F, Lervik A, Bresme F
Non equilibrium molecular dynamics simulations of the thermal conductivity of water: a systematic investigation of the SPC/E and TIP4P/2005 models
Journal of Chemical Physics, 01/01/2012, 137, 74503–74503
Igaluer S, Mathew MS, Bresme F
Molecular dynamics computations of brine-CO2, interfacial tensions and brine-CO2-quartz contact angles and their effects on structural and residual trapping mechanisms in carbon geo-sequestration
Journal of Colloid and Interface Science, 14/07/2012, 386, 405–414
Bresme F, Römer F
Molecular Heat transport in liquid water at extreme pressures: A non equilibrium molecular dynamics study
Journal of Molecular Liquids, 22/10/2012

Dr George Britovsek (CAM)

Dr George Britovsek’s current research projects involve the design and application of homogeneous catalysts in a number of industrially important reactions, including oxidations, carbonylations and polymerization reactions.

IN THE AREA OF ALKANE OXIDATION, TWO STRATEGIES ARE INVESTIGATED:
• Non-heme iron based catalysts serve as bio-inspired catalysts which, in combination with hydrogen peroxide, are capable of oxidizing unfunctionalised alkanes with remarkable activities and selectivities, probably due to the formation of high valent iron oxo intermediates.
• Late transition metals such as platinum are well known for their C-H activating abilities, even unreactive alkanes may be activated in this way. Current research involves the study of the reaction of platinum alkyls with oxidants such as hydrogen peroxide and dioxygen, in particular photocatalytic dioxygen insertion reactions and C-H activation studies.

OTHER AREAS OF RESEARCH ARE:
• The carbonylation of methanol to acetic acid, including the application of carbonylation catalysis to other substrates
• The polymerization and oligomerisation of alkenes

2012 Publications
Smit TM, Tomov AK, Britovsek GJP, Gibson VC, White AJP, Williams DJ
The effect of imine-carbon substituents in bis(imino)pyridine-based ethylene polymerisation catalysts across the transition series
Catalysis Science & Technology, 01/01/2012, 2, 643–655
Nobbs JD, Tomov AK, Cariou R, Gibson VC, White AJ, Britovsek GJ
Thio-Pybox and Thio-Phebox complexes of chromium, iron, cobalt and nickel and their application in ethylene and butadiene polymerisation catalysis
Dalton Transactions, 29/03/2012, 41, 5949–5964
Karpiniec SS, McGuinness DS, Britovsek GJP, Patel J
Acetylene Cyclotrimerization with an iron(II) Bis(imino)pyridine Catalyst
Organometallics, 23/04/2012, 31, 3439–3442
Dr Nicholas Brooks (CB)

Nick Brooks’ research focuses on the effect of high pressure on the structure and micromechanics of biological systems, and dynamic structural changes in soft condensed matter. Coupled to these research aims, Dr Brooks has a strong interest in advanced instrumentation and technique development. He is a leading member of the Membrane Biophysics Platform and Programme Manager of the ‘Sculpting Dynamic Amphiphilic Systems’ Programme, a large scale collaborative project run with Professor John Seddon, Dr Oscar Ces, Dr Rob Law and Professor Richard Templer at Imperial and colleagues at the Universities of Durham, Cambridge, Nottingham and Leeds.

CURRENT RESEARCH OVERVIEW

Hydrostatic pressure is both highly important in the biology of deep sea organisms and as a physical and tool which can be used as a rapid structure change trigger. Pressure can induce a vast range of structural changes in soft matter and biological systems from controlling protein folding to inducing phase changes in model membranes which mimic vital cellular processes. In fact any change that involves a volume reduction can be promoted by pressure. In contrast to other structure change triggers such as temperature, pressure can be changed very quickly and equally fast both up and down; fast pressure-jumps (around 5 ms) allow the thermodynamic trigger to be decoupled from many structural changes and by combining pressure-jump technology with fast structure probe techniques we can study a wide range of dynamic out-of-equilibrium structural behaviour.

Despite great advantages over other structure change initiators, high pressure remains underutilised, primarily due to its technical difficulty. To address this, we have developed two user friendly pressure-jump platforms: (1) Within the Membrane Biophysics Platform, we have developed a pressure-jump system for small and wide angle X-ray diffraction in collaboration with Diamond Light Source. This system is now based at beamline I22 at Diamond and is freely available to beamline users. (2) We have recently extended this technology to develop a versatile pressure jump microscopy platform allowing in-lab access to time resolved high pressure structural studies. This unique platform offers 2-dimensional imaging with high temporal resolution using a range of advanced microscopy techniques including polarised light and fluorescence imaging.

These versatile high pressure systems have facilitated recent collaborative research projects in fuel technology, cell growth and plant science.

2012 Publications

Cook AG, Wardell JL, Brooks NJ, Seddon JM, Martínez-Felipe A, Imrie CT
Non-symmetric liquid crystal dimer containing a carbohydrate-based moiety
Carbohydrate Research, 01/08/2012, 360, 78–83

Hydrostatic Pressure Effects on the Lamellar to Gyroid Cubic Phase Transition of Monolinolein at Limited Hydration
Langmuir, 11/09/2012, 28(36), 13018–13024

Dr James A Bull (Synthesis)

Dr James Bull’s research focuses on the development of efficient synthetic methods to access compounds of biological importance. Dr Bull currently holds a Career Acceleration Fellowship from the EPSRC. The Bull group is currently undertaking research in the following areas:

Lead-oriented synthesis for medicinal chemistry: Our main focus is the synthesis of novel heterocyclic and small ring derivatives, particularly through the functionalization of the intact rings. Chiral small ring heterocycles offer ideal properties as scaffolds for quality lead compounds or fragments for drug discovery, due to their low molecular weight, desirable physical properties, as well as defined 3-dimensional shape. We are developing methods to access diverse heterocyclic derivatives containing biologically important 4-, and 5-membered ring structures.

Aziridine synthesis: Aziridines are strained 3-membered rings that are important intermediates in synthetic chemistry, as well as providing potential probe molecules to investigate biological systems. We are developing methods for the synthesis of diverse aziridine derivatives from universal intermediates by derivatisation of the intact aziridine ring. Central to our approach is the development of the synthetic applications of organometallic reagents, particularly a-halo metal species. Our understanding is supported by kinetic and computational studies.

Catalytic methods in synthesis: We are developing new catalytic reactions for the derivatisation of complex systems, notably involving transition metal catalysed sp3–sp2 cross coupling reactions. Particularly we focus on the use of more sustainable, inexpensive transition metals as catalysts such as copper and iron salts. We are also developing catalytic methods to address industrially important reactions, through the design of metallic and non-metallic catalytic systems that are efficient, cost effective and environmentally benign.

Target-oriented synthesis: We are interested in the synthesis of target molecules for a variety of applications. This includes biologically active natural or unnatural products as well as the synthesis of fluorescent molecular imaging agents.

Dr Bull began independent research at Imperial in October 2009 as a Ramsay Memorial Research Fellow. In October 2011 he started a research group following the award of a Career Acceleration Fellowship.

2012 Publications

Bull JA
Catalytic Enantioselective Synthesis of Secondary Alkylboronate Building Blocks With and Without Metals
my group we are working on sensing and microanalytical devices with a particular focus on human and animal health. Combining physical measurement techniques (electrochemistry and fluorescence spectroscopy) with microfabricated devices (using photolithography and laser machining with nanolithography) and engineered biomolecules (proteins and aptamers) is a central theme of the work.

Current projects include developing point of care diagnostic devices or minimally invasive implantable sensors for conditions such as diabetes, osteoarthritis and cholestasis of pregnancy as well as therapeutic drug monitoring and infectious disease detection. We are also using our engineered biomolecules as potential cell and tissue imaging agents when conjugated to fluorophores and nanoparticles. Research in this area requires close collaboration with clinical colleagues and a strong focus on translating laboratory demonstrations into devices that can ultimately be manufactured and commercialised.

**2012 Publications**

Maniyam MN, Sjahri F, Ibrahim AL, Cass AEG
*Glycine degradation by immobilized cells of Rhodococcus UKMP-5M Biologia*, 01/10/2012, 67, 837–844

Radomska-Botelho Moniz A, Michelakis K, Trzebinski J, Sharma S, Oliver N, Johnston D, Cass A
*Minimally Invasive Enzyme Microprobes: An Alternative Approach for Continuous Glucose Monitoring* *Journal of Diabetes Science and Technology*, 01/03/2012, 6, 479–480

El-Laboudi A, Oliver NS, Cass A, Johnston D
*Use of microneedle array devices for continuous glucose monitoring: a review* *Diabetes Technology & Therapeutics*, 12/12/2012, 15, 101–115

Tian PY, de Jonge LT, Autefage H, Cass AE, Stevens MM
*Engineered alkaline phosphatase with improved functionality immobilized on bone implant surfaces* *Journal of Tissue Engineering and Regenerative Medicine*, 01/09/2012, 6, 195–195
Cell Analysis (Associate Editor), the Editorial Advisory Panel for Molecular Membrane Biology and the Chemistry Subcommittee of Imperial College Press.

2012 Publications

Child C, Gee A, Long N, Ces O
Measuring non-specific binding of novel PET radioligands to determine structure-activity relationships between NSB and their physiochemical properties
Journal of Cerebral Blood Flow and Metabolism, 01/08/2012, 32

Engineering de novo membrane-mediated protein-protein communication networks
Journal of the American Chemical Society, 26/03/2012, 134, 5746–5749

Hydrostatic Pressure Effects on the Lamellar to Gyroid Cubic Phase Transition of Monolinolein at Limited Hydration

Mak LH, Knott J, Scott KA, Scott C, Whyte GF, Mann DJ, Ces O, Stivers J, Woscholski R
Arylstibonic acids are potent and isoform-selective inhibitors of Cdc25a and Cdc25b phosphatases
Bioorganic & Medicinal Chemistry, 24/05/2012, 20, 4371–4376

Furse S, Brooks NJ, Seddon AM, Woscholski R, Templer RH, Tate EW, Gaffney PRJ, Ces O
Lipid membrane curvature induced by distearoyl phosphatidylinositol 4-phosphate
Soft Matter, 2012, 8, 3090–3093

Goyder MS, Willison KR, Klug DR, de Mello AJ, Ces O
Affinity chromatography and capillary electrophoresis for analysis of the yeast ribosomal proteins
BMB Rep, 01/04/2012, 45, 233–238

Shaw KP, Brooks NJ, Clarke JA, Ces O, Seddon JM, Law RV
Pressure – temperature phase behaviour of natural sphingomyelin extracts
Soft Matter, 01/07/2012, 3, 1070–1078

Elani Y, deMello AJ, Niu X, Ces O
Novel technologies for the formation of 2-D and 3-D droplet interface bilayer networks
Lab Chip, 02/08/2012, 12, 3514–3520

Lanigan PMP, Munro I, Grace Ej, Casey DR, Phillips j, Klug DR, Ces O, Neil MAA
Dynamical hologram generation for high speed optical trapping of smart droplet microtools
Biomedical Optics Express, 01/07/2012, 3, 1609–1619

Professor Donald Craig (Synthesis)

The Craig group’s research activities continue in the area of synthesis methods and natural products total synthesis, specifically of alkaloid target molecules. Ongoing target molecule work is directed towards the synthesis of the macroline-related alkaloids suaveoline and alstonerine, and towards morphine and related structures. This work has led to the uncovering of a series of highly regioselective, stereospecific ring-opening reactions of 1,2,3-trisubstituted aziridines using a variety of sulfur-stabilised carbanions possessing sulfone or thioether functionality. These reactions indicate two different directing effects, arising from the presence of either lithium alkoxide or vinyl substituents on the aziridine ring.

Synthesis methods have focused on the continued development of the decarboxylative Claisen rearrangement (dCr) reaction of allylic tosylacetates and related compounds. In particular, we have studied the ambient-temperature mono-rearrangement of tosylmalonate substrates, and have observed first-order kinetics with a linear free-energy relationship exemplified by a straight-line plot for log(kS/kH) against σ+ for the substituent S. This gave a p value of ca. −2.3, clearly indicative of build-up of positive charge character on the benzylic position of the allylic ester moiety. Other aspects of the dCr reaction currently under development include transannular processes for the synthesis of substituted cyclopropanes and cyclobutanes, ring-closing olefin metathesis of double dCr products to give precursors for the synthesis of structurally novel Cp ligands, and conversion of the same precursors into highly substituted pyridines.

In addition, we are actively investigating dCr reactions which involve dearomatisation of heteroaromatic substrates, and are using the products of these unusual processes for further stereoselective carbon–carbon bond-forming transformations.
Dr Mark Crimmin (CAM)

Our research lies at the interface of inorganic chemistry and organic chemistry. We are interested in the synthesis of new inorganic and organometallic compounds and their application to catalytic reactions that either form or break carbon-hydrogen, carbon-heteroatom or carbon-carbon bonds. While these interests manifest in diverse forms, emphasis is placed on new catalysts derived from main group and rare-earth metals and applications relevant to energy storage.

2012 Publications
Crimmin MR, White AJP
Wittig-olefination via an yttrium-coordinated betaine
Chemical Communications, 03/01/2012, 48, 1745–1747
Zirconocene dichloride catalyzed hydridefluorination of C sp2-F bonds

Dr Rob Davies (Synthesis)

Research interests in the Davies group are primarily focussed upon main-group organometallic and coordination chemistry, but also encapsulate a range of inorganic, organic and organometallic topics. Applications lie in the areas of gas storage and separation (including hydrogen gas fuels tanks and carbon dioxide capture), bio-fuel additives and the development of novel asymmetric synthesis protocols.

An active area of research in the group is the development of new Metal-Organic Framework (MOF) materials. These are microporous 3D-coordination polymers consisting of metal based nodes and organic linking units. These materials are of high interest due to their applications in gas storage technologies (including hydrogen gas for automobile fuel tanks and carbon dioxide for carbon sequestration from the exhaust flues of coal power plants), gas separations and heterogeneous catalysis. Research in the Davies group focuses on the construction of novel MOF materials containing ‘light’ s-block metal centres such as magnesium. These ‘lighter’ materials are particularly attractive for mobile applications where weight is a consideration, for example in H2 storage tanks for hydrogen-powered automobiles. In addition, micro-porous MOF materials built from novel, versatile and robust silicon-based linking units have been investigated in collaboration with Dr P Lickiss.

Additionally, the Davies group have been studying the chemistry of s-block organometallics and their applications and mechanisms of operation in organic synthesis protocols. Although lithium organocuprates are one of the most important reagents for the generation of carbon-carbon bonds via 1,4-addition reactions, their solution structures and mechanisms of operation remain topics of much scientific debate. Dr Davies and his group are interested in the study of these reagents and the development of new homo- and hetero-cuprates with improved reactivity and selectivity (especially enantioselectivity) for applications in organic synthetic protocols. They have recently pioneered the use of new 2D HOESY 1H,1H NMR techniques to study the solution equilibrium of lithium organocuprates and have also reported the first solid-state structural characterisations of Grignard derived organocuprates.

2012 Publications
Davies RP, Patel L, White AJ
Preparations of metal trichalcogenophosphonates from organophosphate esters
Inorganic Chemistry, 05/11/2012, 51, 11594–11601
Bomparola R, Davies RP, Lal S, White AJP
Functionalized Organocuprates: Structures of Lithium and Magnesium Grignard 2-Methoxyphenylcuprates
Organometallics, 26/11/2012, 31, 7877–7883
Davies RP, Lickiss PD, Robertson K, White AJP
An organosilicon hexacarboxylic acid and its use in the construction of a novel metal organic framework isoreticular to MOF-5
CrystEngComm, 01/01/2012, 14, 758 –760

Professor John de Mello (NMD)

Dr John de Mello is a Reader in Nanomaterials, specialising in the experimental and theoretical characterisation of nanoparticles and molecular semiconductors – with particular emphasis on their use in optoelectronic devices. In the area of organic semiconductors, his group focuses primarily on the fabrication, analysis and optimisation of light-emitting diodes and solar cells. A key focus is the development of low cost electrode materials based on conducting polymers and carbon nanotubes which offer attractive alternatives to costly indium tin oxide – the industry standard transparent conductor. Recent work has focused on the development of a powerful new experimental technique for the analysis of organic solar cells which provides deep physical insight into the fundamental processes that govern device operation.

In the area of nanoparticles, his group has pioneered the use of microfluidic reactors for the automation and controlled synthesis of nanoparticles. The technique has been successfully applied to the preparation of numerous metal, metal-oxide and compound semiconductor nanoparticles, including CdS, CdSe, TiO2, Ag, Au and Co. In all cases, microfluidic procedures were found to offer clear advantages over bulk synthesis, most notably the ability to fine-tune the physical properties of the final product and to monitor the real-time growth kinetics of the particles.

Dr de Mello has published 55 papers and three patents and was a co-recipient of the Royal Society’s Brian Mercer Award for Innovation in Nanotechnology in 2006. He was recently appointed an ‘Overseas Talent’ under the Chinese Government’s 111 Brain-Gain programme. He is a cofounder of Molecular Vision Ltd – an Imperial spin-out company specializing in the development of low cost sensors for point-of-care diagnostics; other collaborations include the institute of Materials Research and Engineering in Singapore, GeorgiaTech in Atlanta USA, Ajou University in Korea and the Korea Advanced Nanofabrication Centre.
Ronald Laszlo, one of the group's primary research interests, is to develop renewable, low-cost energy technologies that are now widely considered to be a key challenge for the 21st century. The Durrant group's primary research interest is in the development of new chemical approaches to harnessing solar energy conversion—harnessing solar energy either to produce electricity (photovoltaics) or molecular fuels (e.g., hydrogen). They undertake fundamental scientific studies of new materials and device concepts, aiming to elucidate design principles which enable technological development. Their research is based around using transient laser spectroscopies to undertake photochemical studies of light driven electron and energy transfer reactions. Such studies are undertaken in parallel with device development and functional characterisation, employing a wide range of molecular, polymeric and inorganic materials. Control of materials structure on the nanometer length scale is often essential for efficient utilisation of solar energy, and therefore the nano-morphology and the use of nanostructured materials is a key component of our research. The group’s expertise is focused around photochemistry and physical chemistry. However, their research is very much interdisciplinary, with expertise in the group ranging from protein function and inorganic materials synthesis to device physics. They are fortunate to have many external collaborations, both with academic groups and with industry, enabling them to work closely with colleagues working on innovative materials synthesis, theoretical modeling and practical device development and commercialisation.

Complementing these research activities, Professor Durrant also has a role in coordinating research activities across the College through his position as Deputy Director of Imperial’s Energy Futures Lab, Coordinator of Imperial’s Solar Network and Deputy Director of the Doctoral Training Centre in Plastic Electronics.
Dr Joshua Edel (CP)

Dr Joshua Edel has research activities which fall in the general area of nanobiotechnology with an emphasis on the development of micro and nanofluidic devices for analytical and bio-analytical applications and ultra-high sensitivity optical detection techniques. This area of research covers a broad range of science going from chemistry to physics to engineering. Dr Edel’s expertise includes micro and nanofabrication, sample preparation and handling, laser induced confocal microscopy, total internal reflection microscopy, material processing, surface modification chemistries, and standard semiconductor processing/characterization techniques. Recent key achievements include developing novel detection approaches which utilize the added benefits of nanofluidics to maximize molecule detection efficiencies. For example, Dr Edel’s group has recently developed novel nanofabricated membranes for high-throughput DNA fragment sizing applications and rare event diagnostics. Another research example is in the use of microfluidic devices for high throughput parallel array detection capable of detecting rare cellular and molecular events at the single molecule level. The approach used is analogous to using a computing cluster as opposed to a single computer (i.e. the greater the number of processors in a cluster the quicker the computation time). In Dr Edel’s labs, the processors are replaced with fluidic channels in essence creating a super-fluidic chip.
Dr Matthew J Fuchter
(Synthesis)

Dr Matthew Fuchter is a Senior Lecturer in Synthetic and Medicinal Chemistry. He is also Co-Director of the IC MRes course in Drug Discovery and Development and a Senior Investigator in Cancer Medicinal Chemistry for an anti-cancer drug discovery group, CD3. The Fuchter Group use expertise in chemical synthesis to impact molecular science in chemistry, biology and materials.

Previously, he has been instrumental in the development of new synthetic methods and biological applications of the porphyrin macrocycles (in collaboration with Professor A H Holmes FRS). His research has resulted in the development of a novel Ring-Opening-Metathesis Polymerisation-Capture-Release strategy for the chromatography-free synthesis of a variety of novel unsymmetrical porphyrinyls, the preparation of polymer-supported photooxygenation catalysts, and the conjugation of photoactive porphyrin macrocycles to monoclonal antibodies in the preparation of breast-cancer targeted photodynamic therapeutic agents. He has also developed new synthetic methods in supercritical carbon dioxide, including a mild and efficient batch synthesis of ureas, and a continuous flow procedure for the preparation of diarylethers (in collaboration with Professor A H Holmes FRS).

His current research can be divided into the following three areas:

The Development of Novel Therapeutics
Cancer is a group of diseases characterised by the uncontrolled growth and spread of abnormal cells. Extensive research over the past few decades has uncovered a whole variety of genetic abnormalities contributing to the initiation and progression of cancer, whereby such abnormalities occur through mutations of DNA. More recently however, cellular processes that help determine how, when and where the DNA code is deciphered, have been implicated in the development and spread of the disease. These pathways are known as epigenetic processes.

Deciphering the function of each component of the epigenetic machinery will enhance our basic knowledge and lead to the improved therapy and prognoses of several human diseases, including cancer. Together with biological collaborators, we are involved in several medicinal chemistry programmes towards the development of potent and selective inhibitors of epigenetic gene regulation. Not only will such probes allow investigation of the role of epigenetic events in gene expression, but also how such processes are aberrant in cancer. For example recently, we have identified novel small molecules that induce re-expression of aberrantly genes via reversal of epigenetic silencing and induce inhibition of tumour cell growth in breast cancer cell lines. We are also investigating the use of epigenetic therapies in other diseases such as malaria.

Novel synthesis methodology
The development of clean and efficient synthetic procedures is of key interest to the Fuchter Group. We have recently developed a one-pot synthesis of allylic chlorides from aldehydes utilising a mechanistically novel C-O bond fission process, and have reported a number of total synthetic and semi-synthetic routes to biologically important natural products and analogues. Other ongoing projects within the group include the development and application of novel chiral N-heterocyclic and ‘abnormal’ carbenes, and the replacement of lanthanide salts in selective carbonyl addition and reduction reactions.

The Synthesis and Applications of Helical Aromatic Molecules
Planar-fused aromatic molecules can be rendered helical or spirally coiled due to the inability for conjoined rings to occupy the same plane. These fascinating molecules, termed the helicenes due to their helical architecture, have undergone a surge in interest mainly due to their unique optical and electronic properties, closely associated with their inherent chirality. We are currently developing new, and importantly, asymmetric synthetic strategies for the synthesis of carbo- and heterohelicenes. We are also surveying their use as scaffolds in chemical science, as well as their use as components of organic ‘plastic electronic’ devices.

Dr Fuchter is also a senior medicinal chemistry investigator of a cross-College small molecule cancer drug discovery group (Cancer Drug Design and Development Group – CD3), which utilises key strengths at Imperial including synthetic and medicinal chemistry, protein crystallography/structural biology, molecular pharmacology and imaging, epigenetics and pharmacodynamics, pathology, cancer cell biology and phase 1 new drug development. This group spans the Faculties of Natural Sciences and Medicine, as has the overall aim of developing a pipeline for small molecule anti-cancer drug discovery and development at Imperial. Currently the group has seven cancer targets in drug discovery and development, many of which are at an early hit generation stage. One of the targets however has two lead molecules, one of which delivers unprecedented target selectivity, and the other that is poised to enter phase 1 clinical trials.

2012 Publications

Weimar M, Fuchter MJ
Synthesis of sterically encumbered C10-arylated benzo[h]quinolines using ortho-substituted aryl boronic acids
Organic & Biomolecular Chemistry, 15/10/2012, 11, 31–34

Fuchter MJ, Schaefer J, Judge DK, Wardzinski B, Weimar M, Krossing I
[7]-Helicene: a chiral molecular tweezer for silver(I) salts
Dalton Transactions, 06/06/2012, 41, 8238–8241

Current limitations and future opportunities for epigenetic therapies
Future Medicinal Chemistry, 01/03/2012, 4, 425–446

Fuchter MJ, Weimar M, Yang X, Judge DK, White AJP
An Unusual Oxidative Rearrangement of [7]-Helicene
Tetrahedron Letters, 29/02/2012, 53, 1108–1111

Defining the mechanism of action and enzymatic selectivity of psammaplin A against its epigenetic targets
Journal of Medicinal Chemistry, 26/01/2012, 55, 1731–1750

Malmquist NA, Moss TA, Mecheri S, Scherf A, Fuchter MJ
Small-molecule histone methyltransferase inhibitors display rapid antimalarial activity against all blood stage forms in Plasmodium falciparum
Proceedings of the National Academy of Sciences USA, 24/09/2012, 109, 16708–16713
Dr Ian R Gould (CB)

The main objective of Dr Ian Gould's research is the development and application of Quantum Mechanical (QM) and Molecular Mechanical (MM) methods for accurate theoretical investigations of chemical reactivity in large systems. Dr Gould is interested in investigating systems such as proteins, DNA, electronic materials, homo and heterogeneous catalysts, where bond formation/breakage and/or electronic effects are important. A prime area of activity is in the construction 20 of hybrid QM/MM techniques. Ultimately, it is envisaged that the full spectrum of simulation methods, Monte Carlo (MC), Molecular Dynamics (MD) and Free Energy Perturbation (FEP), will be available within the QM/MM formalism. In addition, he is interested in the general development of electronic structure methods, in particular Density Functional Theory (DFT), the Car-Parrinello (CP) method for simultaneous optimisation of electronic and geometric degrees of freedom, and the application of parallel processing methods.

The Gould Group started to develop and apply the first QM/MM methodologies, based around the AMBER force field, capable of tackling electronic spectroscopic processes in biological systems, in collaboration with Professor Klug. They were the first group to show that it is possible to probe the reorganisation energy, involved in electronic absorbance/emission processes, of large biological systems, e.g. Myoglobin and Liver Alcohol DeHydrogenase. The fundamental ethos of this research has been to provide experimental observables to an accuracy of greater than 90% in an algorithmic and reproducible manner. The group have also shown that MM/MD techniques, when correctly parameterised and implemented, are capable of discerning subtle catalytic/binding motifs in enzymatic systems. They showed a priori that for the protein Lys-U, a dimer, it would exhibit 'half of sites binding' which is extremely time consuming, computationally inefficient and also numerically unstable. Dr Gould's group will be working on the development and implementation of analytical 3rd derivative code to circumvent this bottleneck.

2012 Publications

Bradhaw RT, Aronica PGA, Tate EW, Leatherbarrow RJ, Gould IR 
Mutational Locally Enhanced Sampling (MULES) for quantitative prediction of the effects of mutations at protein-protein interfaces 
Chemical Science, 01/01/2012, 3, 1503–1511

Dickson Cj, Rosso L, Betz RM, Walker RC, Gould IR 
GAFFlipid: a General Amber Force Field for the accurate molecular dynamics simulation of phospholipid 
Soft Matter, 2012, 8, 9617–9627

Rosen SA, Gaffney PR, Spiess B, Gould IR 
Understanding the relative affinity and specificity of the pleckstrin homology domain of protein kinase B for inositol phosphates 
Physical Chemistry Chemical Physics, 2012, 14, 929–936

Dr Jason Hallett (CAM)

Dr Jason Hallett's current research projects involve the design and synthesis of task-specific ionic liquids for applications in catalysis and synthetic chemistry.

APPLICATIONS IN CATALYSIS INCLUDE:

- Design and synthesis of protein-friendly ionic liquids for biocatalysis: these are solvent systems where biocatalytic species (enzymes, whole cell biocatalysts) are stabilised for greater activity and improved stability.
- Ionic liquids for base catalysis: these solvents are designed to be catalytic media for base catalysis. Preferential selectivity between nucleophilic and non-nucleophilic mechanisms is also an area of interest.
- Improved reactant gas solubility for catalytic oxidations and hydroformylations: this involves the design of ionic liquids with physical properties that allow for improved solubility of gases such as O₂, or for the formation of mixed solvent systems with rapid gas transport.
- Others areas of research include the development of methodologies for the prediction of reaction kinetics and solution thermodynamics of ionic liquid and CO₂-expanded liquid systems.
**2012 Publications**

Niedermeyer H, Hallett JP, Villar-Garcia IJ, Hunt PA, Welton T

*Mixtures of ionic liquids*

*Chemical Society Reviews, 13/08/2012, 41, 7780–7802*

Brandt A, Erickson JK, Hallett JP, Murphy RJ, Potthast A, Ray MJ, Rosenau T, Schrens M, Welton T

*Soaking of pine wood chips with ionic liquids for reduced energy input during grinding*

*Green Chemistry, 01/02/2012, 14, 1079–1085*

Mota A, Butenko N, Hallett JP, Correia I

*Application of V<sup>2+</sup>O(acac), type complexes in the desulfurization of fuels with ionic liquids*

*Catalysis Today, 30/11/2012, 196, 119–125*

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**Dr Saif Haque (NMD)**

Dr Saif Haque is a Lecturer and Royal Society University Research Fellow. His research interests lie in the area of solar energy conversion and molecular electronics. The displacement of CO<sub>2</sub> emissions by renewable sources of energy critically depends upon the development of low-cost and widely accessible routes to clean energy generation. Of all the renewable energy technologies, solar energy has the greatest potential as a world power source. The energy of solar irradiation incident upon the earth in one hour is equivalent to the world’s entire annual energy consumption at present (~13TW). For this reason, solar photovoltaic (PV), the direct conversion of sunlight to electricity, is expected to play a significant role in future energy supply. One of the most promising options for the development of low-cost photovoltaic devices is the utilization of molecular (or plastic) semiconductors. Dr Haque’s research focuses on the application of laser based optical spectroscopies to study the photochemistry and physophysical processes in organic solar cells.

CURRENT RESEARCH ACTIVITIES INCLUDE:

- The application of femtosecond (ultrafast) laser spectroscopy to study energy and electron transfer in donor-acceptor organic solar cells
- Self-assembly approaches to control nanomorphology and performance of organic solar cells
- Development and application of inorganic quantum dots as light harvesting materials in photovoltaic devices
- Development of hybrid metal oxide/polymer semiconductor nanostructures for light emitting diode devices

Dr Haque has published >50 research papers in the area of molecular solar cells and is a named inventor on five international patents. His research has been recognized by the award of the 2006 Harrison Memorial Medal by the Royal Society of Chemistry.

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**Professor Nick Harrison (NMD)**

Professor Harrison leads the Computational Materials Science Group within the Thomas Young Centre at Imperial and at the Daresbury and Rutherford Appleton Laboratories. His research interests lie in the area of quantum mechanical modeling of material properties with the aim of discovering new functional materials.

**Modelling and Optimising Solar Adsorbers**

An important determinant in the efficiency of a photovoltaic process is the behavior of the solar adsorber material; specifically the trapping of solar energy as an electronic excitation and the subsequent transport of the electrons and holes to the electrodes. These processes are governed by quantum mechanics and occur in the structurally and compositionally complicated environment of a doped semiconductor with solid-solid or solid-liquid interfaces. A modeling environment is being developed in order to provide a complete theoretical description of the equilibrium composition, structure and electronic structure of solar adsorber materials. The aim is to achieve a reliable prediction of the subsequent adsorption of light and energy transport processes. Initial application to the bulk phase diagram and electronic structure of titania and a number of materials from the Cu(I/Ga)(S/Se) family have been completed.

**Intermediate Band Solar Cells Based On Semiconductor Quantum Dots**

Intermediate band solar cells (IBSC) have been proposed as a potential design for highly efficient photo-voltaic devices. Quantum nanostructures, such as quantum dots (QD), arranged in super-lattice arrays produce a mini-band (IB) that is separated by a region of zero density of states from other states in the conduction band. Efficiency is potentially significantly higher than for a single band gap system as additional absorption from the valence band to the IB and from the IB to the conduction band allows two photons with energies below the energy gap to be harvested in generating one electron-hole pair. A multiscale theoretical model of this system has been developed based on...
first principles simulations and a semi-empirical k.p Hamiltonian. The electronic structure and absorption properties of the IB formed by an InAs/GaAs QD array have been computed as a function of dot size and separation indicating and used to develop stipulations for materials growth by molecular beam epitaxy.

Spin Dependent Transport in Nanostructures
The manipulation of electronic spin for information storage and manipulation is a promising approach to ultra fast and energy efficient computing. The discovery of new materials with tailored spin interactions is aided by a detailed understanding of the quantum mechanical processes underlying spin interactions and spin transport. Calculations, based on hybrid exchange density functional theory, have been performed on a number of materials including pure carbon systems (graphene, peapods and nanotubes), metal-organic magnets such as V and Tb (TCNE), and molecular crystals.

2012 Publications
Risplendini F, Cicero G, Mallia G, Bernasconi L, Harrison N
A quantum-mechanical study of ZnO and TiO2, based DSC
Bulletin of the American Physical Society, 29/02/2012, 57(1)

Mukhopadhyay S, Harrison NM
Influence of background carriers on magnetic properties of Mn-doped dilute magnetic Si
Journal of Magnetism and Magnetic Materials, 01/11/2012, 324, 3748–3753

Liborio L, Chew SC, Harrison N
Atomic structure of the (001) surface of CuGaSe2
Surface Science, 01/02/2012, 606, 496–504

Patel M, Mallia G, Liborio L, Harrison NM
Water adsorption on rutile TiO2(110) for applications in solar hydrogen production: A systematic hybrid-exchange density functional study
Physical Review B, 05/07/2012, 86 (4), 045302

Ahmad EA, Mallia G, Kramer D, Tilei V, Kucernak AR, Harrison NM
Physical Review Letters, 19/06/2012, 108 (25), 259701

Ab initio complex band structure of conjugated polymers: Effects of hydrid density functional theory and GW schemes
Physical Review, 04/06/2012, 8 (85), 235105

Dr Martin Heeney (NMD)
Martin is a Reader in Materials Chemistry and the deputy director of the Centre for Doctoral Training in Plastic Electronics. His research mainly concentrates upon the development and characterisation of functional organic materials, with a focus in conjugated materials which display interesting optoelectronic properties. His group is particularly active in the multi-disciplinary area of organic electronics, and collaborates widely, both within Imperial College London and externally.

Current projects include the investigation of chalcogen containing conjugated polymers, where in a series of publications we demonstrated that the switch of sulfur for selenium can result in significant enhancements in electronic performance and result in some of the best performing ambipolar materials prepared to date. We are currently following up this work with the investigation of tellurium containing polymers.

In the area of organic solar cells, we have continued our studies into the development of novel donor polymers. We have extensively investigated the role of the bridging atom in fused aromatic containing polymers. We have shown that the replacement of silicon with germanium results in a significant improvement in the stability of the monomer to base, enabling polymer synthesis by the more benign Suzuki coupling rather than Stille polycoupled condensation. The heteroatom switch also results in an increase in solar cell performance, and an increase in polymer crystallinity for a number of polymeric systems. We have also been active in the search for electron transporting organic materials. We have shown that oxidised DPP derivatives can be stabilised by the inclusion of four strongly electron withdrawing cyano groups. The resulting material forms highly ordered thin films and demonstrates air stable electron transport with some of the best mobilities reported to date. This work, in collaboration with Professor Thomas Anthopoulos (Department of Physics), also demonstrated the first example of an n-type transistor fabricated from a blend of the active component with an insulating polymeric binder.

2012 Publications
Jamieson FC, Domingo EB, McCarthy-Ward T, Heeney M, Stingelin N, Durrant JR
Fullerene crystallisation as a key driver of charge separation in polymer/fullerene bulk heterojunction solar cells
Chemical Science, 01/01/2012, 3, 485–492

Germaindacenodithiophene based low band gap polymers for organic solar cells.
Chemical Communications (Camb), 08/02/2012, 48, 2955–2957

High-performance ambipolar diketopyrrolopyrrole-thienothiophene/bithiophene copolymer field-effect transistors with balanced hole and electron mobilities
Advanced Materials, 2012, 24, 647–652

Solution-processed small molecule-polymer blend organic thin-film transistors with hole mobility greater than 5 cm²/Vs
Advanced Materials, 10/04/2012, 24, 2441–2446
A selenophene-based low-bandgap donor-acceptor polymer leading to fast ambipolar logic
Advanced Materials, 20/02/2012, 24, 1558–1565

Fei Z, Kim Y, Smith J, Buchaca Domingo E, Stingelin N, McLachlan MA, Song K, Anthopoulos TD, Heeney M
Comparative Optoelectronic Study between Copolymers of Peripherally Alkylated Dithienoisoazole and Dithienogermole
Macromolecules, 01/01/2012, 45 (2), 735–742

Factors Governing Intercalation of Fullerences and Other Small Molecules Between the Side Chains of Conducting Polymers Used in Solar Cells
Advanced Energy Materials, 01/10/2012, 2, 1208–1217

Tsai WC, James DT, Domingo EB, Kim JS, Al-Hashimi M, Murphy CE, Stingelin N, Heeney M, Kim JS
Effects of a heavy atom on molecular order and morphology in conjugated polymer:fullerene photovoltaic blend thin films and devices
ACS Nano, 29/10/2012, 6, 9646–9656

Low band gap selenophene-diketopyrrolopyrrole polymers exhibiting high and balanced ambipolar performance in bottom-gate transistors
Chemical Science, 01/01/2012, 3, 181–185

Air-stable and high-mobility n-channel organic transistors based on small-molecule/polymer semiconducting blends
Advanced Materials, 18/05/2012, 24, 3205–3211

Photoconductivity anisotropy study in uniaxially aligned polymer based planar photodiodes
Organic Electronics, 01/01/2012, 13, 36–42

Xia R, Al-Hashimi M, Tsai WC, Heeney M, Bradley DDC, Nelson J
Fused pyrrolo[3,2-d;4,5-d’]bis-thiazole-containing polymers for using in high-performance organic bulk heterojunction solar cells
Solar Energy Materials and Solar Cells, 01/01/2012, 96, 112–116

Brondijk JJ, Maddalena F, Asadi K, van Leijen HJ, Heeney M, Blom PWM, de Leeuw DM
Carrier-density dependence of the hole mobility in doped and undoped regioregular poly(3-hexylthiophene)
Physica Status Solidi B-Basic Solid State Physics, 01/01/2012, 249, 138–141

Thiophene fluorination to enhance photovoltaic performance in low band gap donor-acceptor polymers
Chemical Communications (Camb), 08/10/2012, 48, 11130–11132

A Systematic Approach to the Design Optimization of Light-Absorbing Indenofluorene Polymers for Organic Photovoltaics
Advanced Energy Materials, 01/02/2012, 2, 260–265

Polymer-fullerene miscibility: a metric for screening new materials for high-performance organic solar cells
Journal of the American Chemical Society, 26/09/2012, 134, 15869–15879

Charge photogeneration in donor/acceptor organic solar cells
Journal of Photonics for Energy, 01/01/2012, 2

Factors Governing Intercalation of Fullerences and Other Small Molecules Between the Side Chains of Conducting Polymers Used in Solar Cells
Advanced Energy Materials, 05/09/2012, 24, 6071–6079

Photovoltaic and field effect transistor performance of selenophene and thiophene diketopyrrolopyrrole co-polymers with dithienothiophene
Journal of Materials Chemistry, 01/01/2012, 22, 12817–12823

Kim JS, Fei Z, James DT, Heeney M, Kim J-S
A comparison between dithienoisoazole and dithienogermole donor-acceptor type co-polymers for organic bulk heterojunction photovoltaic devices
Journal of Materials Chemistry, 01/01/2012, 22, 9975–9982

Dr Mimi Hii (CAM)

Mimi Hii is a Reader in Catalysis. Her research interests are in the development of catalytic methodologies for the synthesis of organic molecules; particularly, transition metal catalysts for C-C and C-X bond formations. Working at the interface of inorganic and organic chemistry, her research includes aspects of synthetic, coordination and catalytic chemistry, as well as asymmetric synthesis and mechanistic investigations.

A key focus of her work has been the development of practical and ‘green’ catalytic methodologies; specifically, catalytic O-H and N-H additions to C≡C bonds. Her research group pioneered the use of dicationic palladium(II) catalysts for highly enantioselectiveaza-Michael reactions, which remains the most practical and selective system developed to date. This provided the methodology to develop the synthesis of number of biologically active molecules that are particularly important to the pharmaceutical industry.

Other catalytic methodologies developed by her research groups include the first reported copper-catalysed hydroamination reaction for the addition of non-nucleophilic sulfonamide and carbamates to 1,3-dienes and vinylarenes. This has been subsequently extended to hydroalkoxylation reactions for the construction of biologically relevant O-heterocycles (benzopyrans, cyclic ethers and lactones). Further discoveries have been made of the unique regioselectivity of metal triflate catalysts in intramolecular hydroalkoxylation reactions, and the first report of a Pd-catalysed enantioselective a-hydroxylation of ketoesters.

Dr Hii also enjoys interdisciplinary research, including recent collaborations with the Department of Chemical Engineering, to elucidate mechanisms of activation/decomposition of palladium catalysts, and the development of novel flow chemistry platforms for organic synthesis.
Dr Tricia Hunt (CP)

Many important chemical reactions occur in a solvent (biological, industrial, technological) making solvents a critical issue. However, when a solute becomes solvated in a molecular liquid the electronic structure changes in ways that are not well understood. The group uses a range of computational methods, from classical MD through to high level quantum chemical, to address this issue, studying the electronic structure of solvents and solvated species at the molecular level. Theoretical developments bridge the gap between (classical and solid state) physics and quantum chemistry, and have offered fresh new insights into the electronic basis of solvation and reactivity in condensed phase molecular liquids.

Group interest focuses on aqueous and ionic liquid (IL) solvents, focusing more recently on ionic liquids. Ionic liquids remain fluid down to room temperatures (typically < 100°C), and as a class exhibit unusual physical properties; vanishing vapour pressure, large liquidus range, high thermal stability, high ionic conductivity, high electrochemical stability, and a favourable solvation behaviour. Ionic liquids can outperform traditional solvents, and are being pursued as novel solvents in areas as disparate as industrial catalysis, bio-fuel production, nuclear waste reprocessing, and clean metal electrodeposition. As green replacements for volatile organic compounds (a major source of environmental pollution), ionic liquids can make a significant environmental impact in cleaning up and making more sustainable many industrial processes. Because ionic liquids facilitate catalytic reactions and electrochemical processes at lower temperatures energy consumption is substantially reduced. Ionic liquids can be non-volatile safe green solvents and are primed to replace more dangerous volatile organic solvents in a number of electrochemical devices which are important in our increasingly energy-constrained future, examples include; Li metal batteries, capacitors, hydrogen fuel cells, and photovoltaic cells. Ionic liquids have also seen development as performance chemicals, advanced functional materials and engineering fluids (storage media, fuels and lubricants) and are tipped to make key contributions in the automotive, oil and gas, bio-fuels, battery, textile, construction, and energy industries in the near future.

A second key area of research follows a unified approach to the characterisation and development of catalytic processes, whereby closely interwoven synthetic and computational studies are used to produce real advances. Computational studies fed into catalyst development, which are then employed in targeted organic synthesis or polymer production. One project includes the development of calcium catalysts for inter-molecular hydroamination that are employed to synthesise pharmacologically active alkaloids (used to control bleeding, treat migraine, alleviate pain). A second project includes the development of yttrium catalysts for lactide ring-opening polymerisation to be employed in the production of bio-degradable polymers (used as packaging, fibres or in medicine where a degradable matrix is required) from renewable resources (corn or sugar beet).
can be improved by rational design.limitations in efficiency of metal oxide photocatalysts so that they
efficient hydrogen production. The group is undertaking detailed
driven water splitting by photocatalysts as a means of clean and
used to make high energy fuels. The group are investigating solar-

Hydrogen is a potential fuel of the future or a reagent that can be
for higher plants to be particularly efficient at biomass production.
partly because there is not a great deal of evolutionary pressure
efficiencies closer to the theoretical limit of ~6 per cent. This is
photosynthesis is only 1 per cent efficient, yet algae can achieve
emerging economies and population growth. Higher plant natural
a combination of climate change, economic development of

Natural and Artificial Solar Energy Conversion: There is a pressing

Single Cell Proteomics allows the study of cell to cell variation and
thus an analysis of the stochastic processes that underlie protein levels and their network functions in living cells. These
fluctuations can contain information relevant to the overall cell behaviour and also to the robustness of signalling networks. The
sensitivity that allows us to study individual cells can also be put to good use in diagnostic applications in biomedical research and is a useful by-product of the basic scientific research that drives the development of this technology.

Platform Technologies for the study of Proteomics and Protein-Protein Interactions: There is a tremendous need for better,

Coherent Two-Dimensional Infrared Spectroscopy: 2DIR is an

DNA biophysics
Theory of homology recognition well. From well to a funnel
A theory of the potential well, which traps homologous genes in homology-to homology juxtaposition was developed. The
shape of the well is quasi-exponential with a half-width equal to the earlier introduced homology recognition well (which enters
the expression for the recognition energy, and has now been evaluated by us from independent X-ray experiments as equal to 8f100 Å, the depth of the well is equal to the earlier calculated recognition energy. First variant of the theory, developed in approximation of rigid molecules, gave a fully analytical formula; this year it was extended to the case of torsionally-flexible molecules where result is mathematically more complicated but still fully tractable. They justify the concept of recognition funnel with the ‘recognition reaction moving along a three dimensional potential hypersurface. This theory gives a solid framework to the future single molecule experiments for the measurements of the recognition force trapping two homologies in direct juxtaposition.

**X-ray scattering from DNA with account for sequence-dependent distortions and undulations. A new framework for classical data in DNA fibres**

This was a development of a previously obtained new formalism for X-ray scattering structure factors with account for twist angle and other distortions, on top of which we allowed long wave-length undulations. This completes a new theory for the treatment of X-ray diffraction for wet DNA fibres. Application of this theory gives new information about an adaptable DNA structure under crowded conditions in fags and sperm heads.

**Investigation of the role of undulations on DNA helix-specific forces**

A sophisticated theory has shown a dramatic amplification of helix specific forces due to undulations that were considered earlier less important as being long wave length. In fact, undulations not only influence pre-exponential factors of the DNA-DNA interaction potential, but may renormalize the decay length. Together with undulations taken into account, the calculated DNA osmotic force isotherms look even closer to experimental ones, giving further support to Kornyshev-Leikin theory of DNA-DNA interactions in solutions.

**Electrovariable optics and soft-matter micro- and nano-devices**

**Soft electrified interfaces, electrovariable optics and nanoplasmonics**

**Electrowetting with Interfaces of Immiscible Electrolytic Solutions (ITIES).**

Deeper insight into the understanding of electrowetting with ITIES, with account of a number of effects, coupled to contact angle hysteresis and pulsing-assisted electrowetting dynamics.

**Localisation of nanoparticles at ITIES**

Previous theory of electric-field-induced interfacial localisation of small nanoparticles was extended on the case of large nanoparticles. A model adsorption-desorption isotherm of nanoparticles was derived which gives a framework for understanding the statics and dynamics of nanoparticle field-controlled adsorption-desorption. A theory of light reflection from a layer of nanoparticles of different surface coverage was developed, which describes the electric-field induced conversion of the surface from a transparent state to almost a prefect mirror. This result opens new perspectives for realization of a new generation of self-assembled electrotunable smart windows, mirrors, and optical switches (a patent application was filed). First experimental results approving the predictions of the theory have been obtained in EPFL; a systematic experimental research along the lines of the developed theory has been started in the groups of Professor A Kucernak and Dr J Edel.

**Sustainable energy**

**Double layer in ionic liquids**

Our previous studies of the structure of the electrical double layer and capacitance at the electrode/room temperature ionic liquid interface were based on molecular dynamic simulations of model systems. They have basically reproduced a set of universal predictions of the mean-field theory published AAK in a renowned 2007 feature article, including (i) the capacitance behaviour at high voltages, (ii) the asymmetry of the capacitance curve which follows from the asymmetry in the sizes of cations and anions, (iii) the bell shape of the capacitance for dense ionic liquids, and (iv) the double-hump ‘camel’ shape of capacitance for highly porous ionic liquids. In 2009 investigation was accomplished of the role of elongated shapes of the constituent ions on the double layer capacitance. By means of Monte Carlo simulations it was shown that the camel shape, frequently observed experimentally, may take place also in very dense ionic liquids but with long neutral tails of ions. The tails appear to play the role of latent voids for charge rearrangements, which warrants this spectacular shape.

**2012 Publications**

Cortini R, Lee DJ, Kornyshev A

*Chiral electrostatics breaks the mirror symmetry of DNA supercoiling*  
Journal of Physics Condensed Matter, 30/03/2012, 24, 162203

Kondrat S, Perez CR, Presser V, Gogotsi Y, Kornyshev AA

*Effect of pore size and its dispersity on the energy storage in nanoporous supercapacitors*  
Energy & Environmental Science, 01/04/2012, 5, 6474–6479

Turek V, Cecchini MP, Paget J, Kucernak AR, Kornyshev AA, Edel JB

*A Plasmonic Ruler at the Liquid-Liquid Interface*  
ACS Nano, 01/10/2012, 6(9), 7789–7799

Kornyshev AA, Marinescu M, Paget J, Urbakh M

*Reflection of light by metal nanoparticles at electrodes*  
Physical Chemistry Chemical Physics, 10/01/2012, 14, 1850–1859

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**Professor Anthony Kucernak (CP)**

Professor Anthony Kucernak’s contributions may be grouped into three different areas, (a) the development of innovative new techniques to probe the understanding of electrochemical energy systems; (b) the development of underpinning theory and knowledge as to how electrochemical energy systems operate; and (c) the synthesis of new materials and configurations for electrochemical energy systems by the application of the information gained in (a) and (b).

**Development of new techniques**

Professor Kucernak has developed a number of new approaches to study electrochemical systems of importance to electrochemical energy systems. He has developed electrochemical scanning probe microscopy approaches to study isolated clusters of catalysts deposited on surfaces. This approach allowed *in situ* identification of highly active catalyst particles. This leads to the concept of studying single isolated particles, which was achieved by developing ultra-small nm-sized electrodes, onto which single nm-sized catalyst particles could be reproducibly deposited. This work not only allowed the study of the growth of individual nanoparticles, but also set the scene for studies of individual catalyst particles. He has also developed techniques which allow
the modification of the surface composition of catalysts. This approach allows a deeper understanding of the required surface composition of highly active catalysts. A separate strand of work has involved developing techniques which allow the study of materials under realistic operating conditions. Thus he was the first to provide methods for studying catalysts under true fuel cell conditions, and more recently this has been extended to a much wider range of conditions. At the larger level, he has developed key approaches for understanding the current and reactant distribution within operating fuel cells. The significance of this work is in developing tools to enable us to understand what is really happening in these electrochemical systems.

Improved understanding of electrochemical energy systems. Professor Kucernak has published extensively on the development of kinetic models for understanding processes occurring within fuel cells and other electrochemical systems. This includes details associated with oxidation of fuels and the reduction of oxygen.

Synthesis of new catalysts and development of new systems. Professor Kucernak's work also involves the understanding and development of new materials. Examples of this include the development of new materials for supercapacitors and the development of new catalysts for fuel cells.

2012 Publications


Kucernak A, Bidault F, Smith G. Membrane electrode assemblies based on porous silver electrodes for alkaline anion exchange membrane fuel cells. Electrochimica Acta, 01/11/2012, 82, 284–290


Turek V, Cecchini MP, Paget J, Kucernak AR, Kornyshev AA, Edel JB. A Plasmonic Ruler at the Liquid-Liquid Interface. ACS Nano, 01/10/2012, 6(9), 7789–7799


Dr Marina Kuimova (CP)

Marina Kuimova's research is funded by the EPSRC Career Acceleration Fellowship. The work is concerned with visualising intracellular events and environment using combination of imaging approaches. The research activities can be grouped into three major topics:

Photodynamic Therapy of cancer (PDT)

PDT is a clinically tested promising technique to treat cancer. PDT uses red light to activate light-sensitive drugs (photosensitizers) to produce short lived cytotoxic species such as singlet oxygen to destroy malignant cells. In collaboration with Professor Harry Anderson's group at Oxford we have recently designed efficient sensitizers for two-photon excited PDT, where light induced damage can be precisely localised to a focal point of the pulsed laser. Thus TPE PDT can benefit the treatment of sensitive tissues, where out-of-focus damage should be minimised.

Molecular rotors

Novel fluorescent probes, called molecular rotors, have been developed to image microscopic viscosity inside live cells during normal cell cycle and photodynamic therapy of cancer. Measuring viscosity with high spatial resolution in a cell is important since it controls the rate of diffusion and can affect vital biochemical reactions, signalling and transport. In PDT viscosity determines how far short-lived cytotoxic agents can diffuse before they deactivate, hence, how wide-spread is the light-activated cell damage.

Imaging singlet oxygen

This work is concerned with monitoring the cellular distribution and reaction rates of the most important cytotoxic PDT species, singlet molecular oxygen, in single live cells. These studies can provide an interesting insight into diffusion processes in live cells, complementary to molecular rotors described above. Singlet oxygen work is conducted in collaboration with the group of Professor Peter Ogilby (Aarhus, Denmark)

Prizes

Harrison-Meldola Prize, Royal Society of Chemistry, 2012
The Young Investigator Award, British Biophysical Society, 2012

2012 Publications

Kuimova MK. Molecular rotors image intracellular viscosity. Chimia (Aarau), 01/01/2012, 66, 159–165


Kuimova MK. Mapping viscosity in cells using molecular rotors. Physical Chemistry Chemical Physics, 17/07/2012, 14, 12671–12686

Dr Rob Law (CB)

Solid State NMR Studies of the Liquid Ordered Phase

Recently there has been much interest and controversy in the literature concerning the nature of discrete plasma membrane (PM) micro-domains that may occur in phospholipid (PL) bilayers, commonly called ‘lipid rafts’. Lipid rafts were reported by Simons and Ikonen and they have attracted a great deal of interest because they have been thought to be a separate liquid crystalline phase – the liquid ordered phase ($L_{o}$) phase – present in the fluid ($L_{f}$) liquid crystalline phase of the PM. Lipid rafts have been associated with many fundamental cell processes that are essential for cell growth and survival. It is thought that their role is to recruit specific proteins that allow them to aggregate in these ‘hot spots’ so that they interact with other proteins in these domains to carry out specific functions e.g. signalling processes. Indeed, it is increasingly thought that they...
also play many other fundamental roles in cellular function e.g. invagination processes (‘budding’), infection.

One possible explanation for the existence of lipid rafts has been postulated is due to their molecular composition of sphingolipids e.g. sphingomyelin and cholesterol. Between these molecules, the existence of unusually strong hydrogen bonding gives rise to the tight packing in the Lo phase. Both sphingolipids and cholesterol can occur in high concentrations in the PMs with cholesterol being up to 50 mol% in some types of PM. However, the hypothesis of lipid rafts is problematic in two fundamental ways i) the size of the lipid raft domains and ii) the timescale of their existence. If there are purported to exist in living cells and are due to a lipid-lipid interactions then there would be a line tension between the two phases and therefore they would aggregate to reduce the line tension and be readily visible. Moreover, from many spectroscopic and diffusion studies, the size of the domains must be very small (<10nm). The timescale of their existence has also not been investigated, even if they do exist it is uncertain as to whether they exist on a long enough timescale to significantly influence biological processes. There have been no rigorous biophysical determinations of the structure of lipid rafts and exactly what the relationship of lipid rafts is to the Lo phase is still undetermined.

Using solid state ²H NMR spectroscopy it is possible to determine a very characteristic Pake powder pattern of the liquid crystalline phase present in the bilayer, therefore it will be possible to establish the presence and quantity of the Lo phase in the presence of the Le phase. This can be combined with studies of other nuclei e.g. ¹H, ¹³C, ¹⁴N and ³¹P. The other nuclei give complementary information about the phases present in the bilayer e.g. static ³¹P powder patterns. Furthermore, using the model membranes it is possible to more accurately determine the role of cholesterol and how it contributes to the formation of the Lo phase and how this changes with lipid (particularly sphingomyelin) and cholesterol concentration. Cholesterol can also be specifically deuterated and its interaction with the lipid component e.g. hydrogen bonding, investigated in model membranes and related to the formation and composition of the Lo phase.

**Solid State NMR Studies of the Fluoroaluminosilicates**

The role of fluorine in aluminosilicates is still far from understood. Using ¹⁹F Magic Angle Spinning (MAS) it is possible to determine the structural role that fluorine has within the inorganic glass matrix. This is important as these ceramics form the basis of a wide variety of bioactive dental systems. These systems can, with judicious choice of composition, actively generate fluoroapatite, a mineral that readily forms on the surface of teeth. The glass is an amorphous inorganic material based upon SiO₂-Al₂O₃-P₂O₅-CaO-CaF₂. One of the few methods to give a useful insight into the structure of these materials is MAS NMR. This is able to probe, at an atomic level, the nearest neighbour and next-nearest-neighbour which, in turn, gives the structural information required of the amorphous materials. Conventional techniques are not able to provide this level of detailed information. These materials also form the basis of bioactive ceramics, which can actively regenerate bone. The mechanism by which this occurs is not fully understood but is directly related to the composition and structure of the glass employed. Other ceramics compositions are either rejected by the body or simply become passive and rendered inert. Bioactive ceramics represent a novel system that stimulates regeneration over replacement. What is special about the structure of these glasses is still not fully understood and why it can elicit this biological response is not fully understood. MAS NMR is one of the few methods available that is able to give an insight into the structure of these materials.
to enable manipulation of the process by rational design. By doing so, enzymes’ and receptors’ activities can be modulated either to enable interpretation of the underlying biology, or pharmaceutical intervention in specific processes. The group is particularly interested in molecular recognition that involves interfaces between large protein molecules—these protein-protein interactions play extremely important roles in biology and it is hoped that disrupting these forces in a targeted manner will offer a fruitful avenue for therapeutic intervention.

This research involves a range of techniques spanning synthetic chemistry through to enzymology; the group employs both molecular biology and solid-phase peptide synthesis to produce modified proteins, high throughput screening and traditional synthesis to find inhibitors, quantitative inhibition kinetics to define the potency of inhibitors, and structural biology to investigate the underlying basis of the activity.

Synthetic Proteins: Professor Leatherbarrow’s group uses automated solid-phase peptide synthesis to create constrained protein mimics, small proteins and protein analogues. They have recently been particularly interested in the synthesis of the cyclic protease inhibitor protein MCotI-II, which is one of the most potent known inhibitors for this class of enzyme. They have described the first chemical synthesis of this protein, and made a large number of analogues which redirect activity towards a number of different protease enzyme targets.

Enzyme Inhibitors: Professor Leatherbarrow’s group has programmes to discover novel, potentially therapeutic, inhibitors for a number of enzyme targets. Of particular note are the 3C protease enzyme from the Foot-and-Mouth Disease Virus, where group members have defined the enzyme’s substrate specificity and generated novel mechanism-based inhibitors, and N-Myristoyl Transferase from Plasmodium falciparum (the causative agent of malaria) where they have identified potential lead inhibitors which have described the first chemical synthesis of this protein, and made a large number of analogues which redirect activity towards a number of different protease enzyme targets.

Protein Labelling: Professor Leatherbarrow’s group employs modern chemical biology methods to allow bio-orthogonal protein tagging, using the Staudinger-Bertozzi ‘click’ reactions to introduce a range of tags onto proteins.

2012 Publications


Discovery of Novel and Ligand-Efficient Inhibitors of Plasmodium falciparum and Plasmodium vivax N-Myristoyltransferase

Journal of Medicinal Chemistry, 17/12/2012, 56, 371–375

Offermann DA, McKendrick JE, Sejberg JJ, Mo B, Holdom MD, Helm BA, Leatherbarrow RJ, Beavil AJ, Sutton BJ, Spivey AC

Synthesis and incorporation into cyclic peptides of tolan amino acids and their hydrogenated congeners: construction of an array of A-B-loop mimetics of the Cε3 domain of human IgE

Journal of Organic Chemistry, 07/03/2012, 77, 3197–3214


Design and synthesis of inhibitors of Plasmodium falciparum N-myristoyltransferase, a promising target for antimalarial drug discovery

Journal of Medicinal Chemistry, 03/10/2012, 55, 8879–8890


Selective inhibitors of protozoan protein N-myristoyltransferases as starting points for tropical disease medicinal chemistry programs

PLoS Neglected Tropical Diseases, 24/04/2012, 6

Bradshaw RT, Aronica PGA, Tate EW, Leatherbarrow RJ, Gould IR

Mutational Locally Enhanced Sampling (MULES) for quantitative prediction of the effects of mutations at protein-protein interfaces

Chemical Science, 01/01/2012, 3, 1503–1511


Discovery of Plasmodium vivax N-myristoyltransferase inhibitors: screening, synthesis, and structural characterization of their binding mode

Journal of Medicinal Chemistry, 22/03/2012, 55, 3578–3582

Dr Paul Lickiss (Synthesis)

The Lickiss group continues to work in several areas of organosilicon chemistry, the synthesis and characterisation of metal-organic frameworks as materials for hydrogen storage, and the use of siloxanes as solvents. In addition, the applications of ultrasound to synthetic chemistry continue to be investigated. The group has also started to work in the area of drug syntheses aiming to make photodynamic therapy drugs that are specifically able to conjugate onto proteins applied to cancer therapy.

Organosilicon Chemistry

We continue to work with Professor T Welton on a study of the potential of methylsiloxanes such as (Me3Si)2O and (Me2SiO)4 as solvents in which chemical processing may be carried out. Fundamental solvent parameters have been measured and a range of reactions have been carried out in the solvents in order to assess their stability and their potential to replace more traditional volatile organic solvents for synthesis. Gas-phase structural studies of polyhedral silsesquioxanes such as Si10O15H10 and Si8O12Ph8 (see figure below), continue with Dr D Wann (Edinburgh) and with Dr S Masters (Canterbury, NZ) in order to gain experimental data that can be compared directly with the many theoretical studies on these widely used compounds.

The gas-phase structures of Si8O12Ph8 (above left), and the D4 symmetry conformer of Si10O15H10 (above right).

(Received atoms are oxygen, yellow or blue are silicon, black are carbon, and white, hydrogen.)

[Image 35x190 to 106x785]
Metal-Organic Frameworks for Gas Storage

We have extended our work in this area and continue to work in collaboration with Dr R Davies. We have used both more traditional organic heterocycles as linkers between metal nodes and have also prepared novel silsesquioxanes and other siloxane based molecules to act as ligands at metal centres of the formation of framework materials. We have made several new porous materials that have a high surface area, such as shown below, and which can absorb hydrogen, including a manganese complex containing a bis-imidazole based linker. The hydrogen uptake studies are being carried out via a collaboration with The University of Birmingham.

A metal organic framework similar to the well known MOF5 but containing a hexa-acid organosilicon ligand connecting zinc(II) centres. The yellow sphere represents a pore of ca. 1.35 nm diameter. (Red atoms oxygen, green silicon and black carbon, blue tetrahedral zinc, hydrogen atoms omitted.)

2012 Publications

Bulut S, Ab Rani MA, Welton T, Lickiss PD, Krossing I
Preparation of [Al(hfp)]-based ionic liquids with siloxane-functionalized cations and their physical properties in comparison with their [Ti,N]-analogues
ChemPhysChem, 12/03/2012, 13, 1802–1805

Davies RP, Lickiss PD, Robertson K, White AJP
An organosilicon hexacarboxylic acid and its use in the construction of a novel metal organic framework isoreticular to MOF-5
CrystEngComm, 01/01/2012, 14, 758–760

Professor Nicholas Long (CAM)

The Long group specialises in synthetic organometallic and inorganic chemistry for functional molecules. Ligand and complex design is crucial and elegant synthetic strategies have been developed, dovetailed with utilisation of the new compounds for applications within catalysis, materials science and biomedical imaging.

Metalloocene chemistry – new ferrocene ligands, transition metal catalysts, redox-active catalysis

The design of novel ligands and metal catalysts has enormous ramifications for chemical syntheses and industrial processes. The work has impact in the understanding of metal-ligand reactivity and the control of industrially-relevant processes such as olefin and lactide polymerisation. In a proof of concept study, the Long group have established for the first time that redox switches may be used to attenuate the activity of single-site polymerization catalysts (J. Am. Chem. Soc., 2006, 128, 7410). Thus, a titanium-based lactide polymerization initiator supported by a ferrocenyl-substituted salen ligand exhibits a substantially higher rate of propagation than its oxidized dicaticonic ferrocenium analogue. The reversibility of the redox event is demonstrated by treatment with redox reagents – and is a rare example of redox-active catalysis.

Organometallic Polymers, Transition Metal- and Metallocenyl-Alkynyl Chemistry

A range of new organometallic metal-alkynyl compounds have been synthesised, and utilised as building blocks for ‘molecular wires’ and as materials possessing electrical conductivity, luminescence and liquid crystallinity. One particular project (in collaboration with Tim Albrecht) examines electrochemical charge transfer in complex molecules. Charge transfer processes in individual molecules and nanoscale structures offer insight into developing ultra-small electronic devices. The project involves the synthesis of multi-centre redox molecules with novel optical, electronic and magnetic properties. Current transport in complex structures is being examined – in branched systems with redox or magnetic centres in parallel.

Biomedical Imaging Agents

This work has significant impact on the design of new imaging agents that are pivotal in the early detection of disease and the evaluation of medical treatment. The Long group are focussing on (i) rapid and efficient syntheses of new ¹¹C-labelled molecules (as ¹³C only has a half-life of 20 minutes), (ii) ‘smart’ optical and MRI contrast agents that have a triggered response and better localisation within the body, (iii) dual-modality imaging probes.

(i) New Strategies for ¹¹C-Labelling in Positron Emission Tomography (PET): From Fast Synthesis to Microfluidics Transition metal-catalysed organometallic processes are being utilised for the formation of ¹¹C-labelled amides, esters and thiesters, forming new transition metal macrocyclic CO/CO₂-containing compounds, and applying the syntheses on a microfluidic scale via ‘lab-on-a-chip’ technology. For the first time a microstructured device has been used to perform a gas-liquid carbonylation reaction – featuring the Pd-catalysed cross-coupling reaction of arylhalides with benzylamine and CO to rapidly form a range of secondary amides. The group are currently (i) designing supported palladium catalysts (incorporating more efficient phosphine ligands) capable of carbonylatve cross-coupling reactions to give high activities and yields with minimal metal leaching; (ii) developing a microfluidic reactor to preconcentrate ¹³CO and a solid-supported palladium catalyst to accelerate the incorporation of ¹³CO into specific molecular probes for PET imaging; (iii) designing the microreactor system to facilitate radiolabelling by other radioisotopes e.g. ¹⁸F. ²⁴¹⁸⁸

(II) Dual-Modality Imaging Probes: By the synergistic combination of two or more detection techniques (such as PET, MRI or optical imaging), we hope to facilitate better reliability and quality of imaging data → earlier detection and characterisation of disease better, more effective treatment. One of the recent examples within the group features the combination of an optical probe (quantum dot or QD) with an MRI centre (gadolinium-containing macrocycle). A range of CdSe/ZnS-capped QDs featuring bidentate phosphine and phosphine oxide ligands as capping species have been formed, with the ligands conferring biocompatibility through solubility and attachment of biomolecules.
The QDs give highly emissive, photostable luminescence and preliminary MRI studies at the Hammersmith Hospital show promising T1-weighted MRI activity. Translation into the clinic and surgery can be envisaged as for example, the probes can guide the scalpel (via fluorescence imaging) and ensure that all the cancerous material has been removed (MR imaging).

Another example features the additional inclusion of a zinc-sensor to these probes, to measure intra- and extra-cellular zinc concentrations. Thus, the probes can monitor, in a safe and non-invasive way, beta cell and insulin release – key factors in the understanding of type I diabetes, facilitating novel therapeutic treatments of this disease.

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**Dr Kevin Lovelock (CP)**

Dr Kevin Lovelock's current research projects involve understanding and predicting ionic liquid properties, primarily through investigating their bulk and surface energetics.

Ionic liquids have been proposed in a wide variety of applications, e.g. electrolytes for batteries and solar cells, solvents for biocatalysis and synthesis, engineering fluids for lubrication and extraction, and in sensors. There is huge scope for further development as ionic liquid properties can be tuned to match the requirements of any particular process. However, only ~10³ ionic liquids out of a possible 10⁶ have been synthesised, and ~20 have been well-characterised. What is lacking is the necessary understanding of ionic liquid properties and ionic liquid-based systems to allow useful predictions.

For ionic liquids, the critical properties (used for predictions of properties of molecular liquids) cannot be accessed experimentally due to thermal decomposition. Therefore, other methods of property prediction are required. Dr Kevin Lovelock's research focuses on developing quantitative relationships between the enthalpy of vaporisation, ∆vapH, and liquid/gas surface tension, g, to allow such predictions. Ionic liquids have very low vapour pressures, similar to metals such as zinc, making measurements of ∆vapH extremely challenging. The quantitative relationships allow predictions of ∆vapH and g for ionic liquids not yet synthesised.

These studies of the liquid phase bulk and surface energetics serve as a platform for the group’s investigations of ionic liquid-based model systems that underpin applications. Currently, the group concentrates on two main areas: understanding the principles of self-assembly of ionic solutes in ionic liquids, which is key to the development of nanostructured functional materials (e.g. ionogels) to be used in transistors, membranes and actuators, and understanding the energetics of ions in confined spaces, which is vital to the development of supercapacitors.

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**2012 Publications**

Child C, Gee A, Long N, Ces O
Measuring non-specific binding of novel PET radioligands to determine structure-activity relationships between NSB and their physiochemical properties
journal of Cerebral Blood Flow and Metabolism, 01/08/2012, 32

Bakewell C, Cao TP, Long N, Le Goff XF, Auffrant A, Williams CK
Yttrium phosphasalen initiators for rac-lactide polymerization: excellent rates and high iso-selectivities
Journal of the American Chemical Society, 26/12/2012, 134, 20577–20580

Tate CW, Gee AD, Vilar R, White AJP, Long NJ
Reversible carbon monoxide binding at copper(I) P-S-X (X=N, O) coordination polymers

Inkpen MS, Du S, Driver M, Albrecht T, Long NJ
Oxidative purification of halogenated ferrocenes
Dalton Transactions, 22/11/2012

Stasiuk Gj, Faulkner S, Long NJ
Novel imaging chelates for drug discovery
Curr Opin Pharmacol, 09/08/2012, 12, 576–582

Gong X, Miller PW, Gee AD, Long NJ, deMello AJ, Vilar R
Gas-Liquid Segmented Flow Microfluidics for Screening Pd-Catalyzed Carboxylation Reactions
Chemistry: A European Journal, 01/01/2012, 18, 2768–2772

Bis(8-quinolinolato)aluminum ethyl complexes: Iso-Selective Initiators for rac-Lactide Polymerization
Organometallics, 09/07/2012, 31, 4729–4736

Kealey S, Plisson C, Collier TL, Long NJ, Husbands SM, Gee AD
Journal of Labelled Compounds & Radiopharmaceuticals, 01/01/2011, 54

Faulkner S, Long NJ
Radiopharmaceuticals for imaging and therapy
Dalton Transactions, 01/01/2011, 40, 6067–6067

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**2012 Publications**

Lovelock KRJ
Influence of the ionic liquid/gas surface on ionic liquid chemistry
Physical Chemistry Chemical Physics, 21/04/2012, 14, 5071–5089

Men S, Hurisso BB, Lovelock KRJ, Licence P
Does the influence of substituents impact upon the surface composition of pyrrolidinium-based ionic liquids? An angle resolved XPS study
Physical Chemistry Chemical Physics, 21/04/2012, 14 (15), 5229–5238
Professor Iain McCulloch (NMD)

Professor Iain McCulloch is Professor of Polymer Chemistry. His appointment commenced in October 2007, with the goal to continue his research in solution processable organic semiconductor materials for application in organic field effect transistors and photovoltaic devices. Prior to his appointment, he was the Research Manager at Merck Chemicals, responsible for the organic electronics programme, encompassing design and development of organic semiconducting materials.

This primarily involved the design of novel organic conjugated aromatic thienothiophene polymers and control of their alignment and organization in the liquid crystalline phase. Understanding relationships between molecular self assembly and charge transport properties resulted in these materials having the largest field effect mobility (1 cm²/Vs) measured in a solution processed OFET device. More recently, solution processable small molecule/polymer blends have also been developed with further improvements in electrical properties. He was co-inventor on over 50 patent families filed from these research activities, and over 70 publications.

2012 Publications


Photovoltaic and field effect transistor performance of selenophene and thiophene diketo-pyrrolopyrrole co-polymers with dithienothiophene base

Journal of Materials Chemistry, 01/02/2012, 22, 12817–12823

Biniek L, Schroeder BC, Nielsen CB, McCulloch I

Recent advances in high mobility donor-acceptor semiconducting polymers

Journal of Materials Chemistry, 01/03/2012, 22, 14803–14813


On the energetic dependence of charge separation in low-band-gap polymer/fullerene blends

Journal of the American Chemical Society, 29/10/2012, 134, 18189–18192


Solution-processed small molecule-polymer blend organic thin-film transistors with hole mobility greater than 5 cm²/Vs

Advanced Materials, 10/04/2012, 24, 2441–2446

Dimitrov SD, Nielsen CB, Shoae S, Tuladhar PS, Du J, McCulloch I, Durrant JR

Efficient Charge Photogeneration by the Dissociation of PC70BM Excitons in Polymer/Fullerene Solar Cells

Journal of Physical Chemistry Letters, 05/01/2012, 3, 140–144


Random benzothiadiazine-based donor-acceptor copolymers for efficient organic photovoltaic devices

Chemical Communications, 01/01/2012, 48, 5832–5834


Design of semiconducting indacenodithiophene polymers for high performance transistors and solar cells

Accounts of Chemical Research, 26/01/2012, 45, 714–722


Use of X-ray diffraction, molecular simulations, and spectroscopy to determine the molecular packing in a polymer-fullerene bimolecular crystal

Advanced Materials, 05/09/2012, 24, 6071–6079


Factors Governing Intercalation of Fullerenes and Other Small Molecules Between the Side Chains of Semiconductor Polymers Used in Solar Cells

Advanced Energy Materials, 01/10/2012, 2, 1208–1217


Silindacenodithiophene-Based Low Band Gap Polymers – The Effect of Fluorine Substitution on Device Performances and Film Morphologies

Advanced Functional Materials, 24/04/2012, 22, 1663–1670


Charge photogeneration in donor/acceptor organic solar cells

Journal of Photonics for Energy, 01/01/2012, 2

Ashraf RS, Kronemeijer AJ, James DI, Sirlinghaus H, McCulloch I

A new thiophene substituted isoindigo based copolymer for high performance ambipolar transistors

Chemical Communications, 25/04/2012, 48, 3939–3941


Photoconductivity anisotropy study in uniaxially aligned polymer based planar photodiodes

Organic Electronics, 01/01/2012, 13, 36–42


Chemical Communications, 11/08/2012, 48, 7699–7701


Correlating Emissive Non-Geminate Charge Recombination with Photocurrent Generation Efficiency in Polymer/Perylene Diimide Organic Photovoltaic Blend Films

Advanced Functional Materials, 06/06/2012, 22, 2318–2326


Germaindenacodithiophene based low band gap polymers for organic solar cells

Chemical Communications, 08/02/2012, 48, 2955–2957


A Systematic Approach to the Design Optimization of Light-Absorbing Indenofluorene Polymers for Organic Photovoltaics

Advanced Energy Materials, 01/02/2012, 2, 260–265
Dr Philip Miller (CAM)

Philip Miller is a lecturer in PET radiochemistry. Positron Emission Tomography (PET) is a clinical imaging technique that uses short-lived positron emitting isotopes to generate a picture of organs and tissues within the body. It is now widely used for the staging of cancer treatment and research into neurodegenerative diseases such as Parkinson’s and Alzheimer’s. PET scans rely on the production of isotopically labelled tracer molecules; C-11 and F-18 being the two most commonly used radioisotopes for PET. A key challenge in this area of chemistry is the rapid synthesis of C-11 and F-18 tracers owing to their short half-lives, 20 and 110 min respectively. Research in the Miller group is directed towards the development of fast and innovative technology to radiolabelling methodology. The group is also investigating fundamental coordination chemistry with P-N donor ligands, flow chemistry and homogeneous catalytic reactions.

Figure 1: Rapid conversion of $^{11}$CH$_3$I to $^{11}$CS$_2$ for PET radiolabelling applications.

**2012 Publications**

Gong X, Miller PW, Gee AD, Long NJ, deMello AJ, Vilar R
Gas–Liquid Segmented Flow Microfluidics for Screening Pd-Catalyzed Carbonylation Reactions
Chemistry: A European Journal, 01/01/2012, 18, 2768–2772

Miller PW, Bender D
$[^{11}C]$Carbon Disulfide: A Versatile Reagent for PET Radiolabelling
Chemistry – A European Journal, 01/01/2012, 18, 433–436

Dr Brian O’Regan (NMD)

The O’Regan group specializes in Dye Sensitized Solar Cells (DSSCs) and related technologies. The overall goal of the group is to combine fundamental characterization, full cell modeling, and in house cell fabrication to allow rational development of more efficient, more stable, and easier to manufacture DSSCs. Finally, our hope is to make a real contribution to renewable energy supplies for the future.

To further these ends we are investigating the materials and mechanisms that underly this technology from the picosecond timescale in the lab out to decades under actual operation. This work involves a wide range of chemical studies and instrumentation. The research activities span the domains of physics, chemistry and engineering. In fabrication and optimization studies, we make cells using different dyes (usually from outside groups), semiconductors (typically oxides such as TiO$_2$) and electrolytes; on metal, glass and plastic substrates. In investigating the initial conditions inside the cell, we use electrochemical and electrokinetic (streaming potential) measurements to measure the interaction of the electrolyte with the dye and meso-porous semiconductor. To investigate the operation of the cell we use transient and steady state electrical characterization to determine the number of electrons, their motion, and their loss to recombination pathways. In recent years we have developed some entirely new transient opto/electronic characterization tools, and revived some languishing steady state techniques. Results from these analyses have allowed us to overturn some long standing ideas about DSSC cell function and best future optimization pathways.

For chemical processes in the cell we use transient absorption spectroscopy to measure rate constants over the 20 ns to 1 second timescale. We also use photo-induced absorption (PIA) to study how the same processes manifest themselves under steady state operation (i.e. delivering power under illumination). To probe faster processes we use luminescence decay measurements (time correlated single photon counting) and collaborations with fs TAS groups. To fully understand individual steps we use the above techniques to find the fundamental rate equations, and the effects of temperature to find the activation energies.

We have developed and and built in-house an instrument that performs a suite of automated characterizations of DSSCs. We use this device in collaboration with both industrial and academic partners to characterize new cell components and designs and also the effect of long term exposure on the cell and its function.

On the modeling side, we have developed a full cell model that runs in Matlab. This model allows us to test ideas about cell function derived from experiments, to check our assertions about the meaning of various experimental signals. The model now needs to be extended to solar cell modules, a transformation from 1 D to 2 D that will be non-trivial.

Cell development activities include the study of DSSC fabrication on less expensive metal substrates, using molecular hole conductors to replace the electrolyte, and water based electrolytes to replace organic solvent presently used.
**2012 Publications**

Xiao Li, Anna Reynal, Piers R. F. Barnes, Robin Humphry-Baker, Shaik. M. Zakeeruddin, Filippo De Angelis, Brian C O'Regan
**Measured binding coefficients for iodine and ruthenium dyes; implications for recombination in dye sensitised solar cells**
*Physical Chemistry Chemical Physics*, 01/01/2012, 14, 15421–15428

**Effect of molecular filtering and electrolyte composition on the spatial variation in performance of dye solar cells**
*Journal of Electroanalytical Chemistry*, 01/01/2012, 664, 63–72

Juozapavicius M, O’Regan BC, Anderson AY, Grazulevicius JV, Mimaite V
**Efficient dye regeneration in solid-state dye-sensitized solar cells fabricated with melt processed hole conductors**
*Organic Electronics*, 01/01/2012, 13, 23–30

Martiniani S, Anderson AY, Law C, O’Regan BC, Barolo C
**New insight into the regeneration kinetics of organic dye sensitised solar cells**
*Chemical Communications (Camb)*, 24/01/2012, 48, 2406–2408

Richards CE, Anderson AY, Martiniani S, Law C, O’Regan BC
**The Mechanism of Iodine Reduction by TiO2, Electrons and the Kinetics of Recombination in Dye-Sensitized Solar Cells**

Miettunen K, Barnes PRF, Li X, Law C, O’Regan BC
**The effect of electrolyte filling method on the performance of dye-sensitized solar cells**
*Journal of Electroanalytical Chemistry*, 15/07/2012, 677, 41–49

O’Regan B, Li X, Ghaddar T
**Dye adsorption, desorption, and distribution in mesoporous TiO2 films, and its effects on recombination losses in dye sensitized solar cells**
*Energy & Environmental Science*, 01/05/2012, 5, 7203–7215

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**Professor Nick Quirke (CP)**

The Quirke group use molecular simulation, theory and experiment to study phenomena at the nanoscale.

Systems of interest include nanofluidic flows, nanoparticles in biofluids and biomembranes for which we aim to elucidate the fundamental chemical physics of particle-environment interactions and transport. Potential applications include nanofluidic devices for medical applications, as well as novel probes of complex biological systems.

Using molecular dynamics we are studying transport of nanoparticles across lung surfactant monolayers to help understand the effect of nanoparticulates on lung function.

In 2008 the group solved a long standing problem in nanofluidics, deriving a novel expression connecting the interfacial slip in a nanopore to the pore width. This expression has been tested using simulation and found to hold for a variety of surfaces (M Groombridge, PhD student, work in progress). Using experiment, the group (in collaboration with Dr M Thanou, King’s College London) produced the first flow measurements for flow through carbon nanopipes (see figures 1,2,3) and reported significantly enhanced flow for polar/non polar fluids. In other work we are following up our suggestion of using Raman scattering to determine water/nanotube interaction potentials and to probe ultra low frequency solvent modified vibrations.

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**Figure 1:** Composite micrograph showing examples of template carbon nanopipe arrays produced in the course of this project using CVD:

a) a bundle of nanopipes partially released from the AAO template following sonication in NaOH
b) cross section of intact carbon coated membrane with highly aligned nanopipe array visible
c) higher magnification view of individual aligned carbon pipes;
d) the surface of the carbon coated AAO template showing open pores (diameter ~ 160 nm)

**Figure 2:** Individual nanopipes (from reference 2)

**Figure 3:** A nanopipe bundle penetrating a cell (work in collaboration with the nanovision centre at QMC – Max Whitby, Ken P’ng, Asa Barber, Joanna Stawiskowska, Maya Thanou and Nick Quirke).

**Figure 4:** Polar nanoparticles translocating DPPC monolayers from the vapour to the water phase. Groombridge M, Schneemilch M, Quirke N.
Professor Mike Robb (CP)

The quantum chemistry group led by Professor Robb is involved in both development of the methodology of quantum chemistry and in applications to non-adiabatic chemistry including photochemical reactivity and electron transfer. Theoretical developments are focussed on non-adiabatic chemistry and some of this work has been released in the Gaussian 9 program suite (see publications). Our applications work involves photochemistry and photobiology.

2012 Publications

Halasz GJ, Perveaux A, Lasorne B, Robb MA, Gatti F, Vibok A
Simulation of laser-induced quantum dynamics of the electronic and nuclear motion in the ozone molecule on the attosecond time scale
Physical Review A, 22/10/2012, 86, 043426–043432

Blancafot L, Robb MA
A Valence Bond Description of the Prefulvene Extended Conical Intersection Seam of Benzene
Journal of Chemical Theory and Computation, 01/12/2012, 8, 4922–4930

Jornet-Somoza J, Lasorne B, Robb MA, Meyer HD, Lauvergnat D, Gatti F
A generalised 17-state vibronic-coupling Hamiltonian model for ethylene
Journal of Chemical Physics, 28/08/2012, 137, 84304

Boggio-Pasqua M, Burmeister CF, Robb MA, Groenhof G
Photochemical reactions in biological systems: probing the effect of the environment by means of hybrid quantum chemistry/molecular mechanics simulations
Physical Chemistry Chemical Physics, 26/04/2012, 14, 7912–7928

Mendive-Tapia D, Lasorne B, Worth GA, Robb MA, Bearpark MJ
Towards converging non-adiabatic direct dynamics calculations using frozen-width variational Gaussian product basis functions
Journal of Chemical Physics, 27/11/2012, 137, 22A538

Serrano-Pérez JJ, Bearpark MJ, Robb MA
The extended S1/S0 conical intersection seam for the photochemical 2+2 cycloaddition of two ethylene molecules
Molecular Physics, 27/06/2012, 110, 2493–2501

Professor Henry Rzepa (Synthesis)

Major advances in four broad areas have been made during this period. In collaboration with the Scheschkewitz group in this department, we have identified an entirely novel form of aromaticity in a small silicon-rich cluster. The dismutational origins of this aromaticity, and the unusual magnetic properties it brings have been analysed with the help of another collaborator. These advances in our understanding of small silicon clusters help put the synthetic work of the Scheschkewitz group on a sound theoretical framework.

Another significant advance has been in exploitation of new theoretical methodologies for computing classes of molecule whose reactions exhibit both covalent and ionic character on the potential energy surface. For example, carbocations as reactive intermediates were famously first proposed by Meerwein in 1924 by way of explanation of the mechanism of the solvolysis of covalent isobornyl chloride. The impact of this advance has been immense; more than 15,000 articles alone have been published in the last 80+ years on this topic. But until our work, it was not possible to utilise a consistent and practical methodology for modelling such mechanisms theoretically. In collaboration with Schleyer (who has spent 55 years working in this area), we revisited isobornyl chloride, and were able for the first time to demonstrate quantitatively accurate models for all the important aspects of this system. In collaboration with Hii in this department we were able to utilise this methodology in improving the understanding of how stereocentlab in a very important catalytic system can be achieved, an important feature of this being the ion-pair that is formed. The methodology also proved crucial in understanding the key features of reactions inside supramolecular cavities, which also involve (in this example four) ion pairs. This work shows that it is now viable to calculate rates of reactions occurring inside such cavities, nowadays a very important area of inter-disciplinary research into catalysis.

Our third area involves developing methodologies for analysing bonding in novel systems. For example, the bonding in the recently discovered species HOSCH, which we identified as having a C-S bond capable of being continuously tuned between triple and single bond character. Tunable bonds is a new concept in bonding theory, and the search for new examples is now under way. Our interest in new methods for characterising aromaticity continues, with an important contribution to a new class of allen-o-acetylenic macrocycles.

Our final area of interest is developing infrastructures for the chemical semantic web. An important article describing the role of digital repositories in this endeavour was published, together with a general review article on the current state.

Prize

ACS Herman Skolnik award for outstanding contributions to and achievements in the theory and practice of chemical information science and related disciplines.
**2012 Publications**

Buchard A, Jutz F, Kember MR, White AJP, Rzepa HS, Williams CK

*Experimental and Computational Investigation of the Mechanism of Carbon Dioxide/Cyclohexene Oxide Copolymerization Using a Dizinc Catalyst*. Macromolecules, 11/09/2012, 45, 6781–6795

Leszczyńska K, Abersfelder K, Majumdar M, Neumann B, Stammler HG, Rzepa HS, Jutzi P, Scheschkewitz D

*The Cp*+R cation as a stoichiometric source of silicon*. Chemical Communications, 04/07/2012, 48, 7820–7822

Braddock DC, Roy D, Lenoir D, Moore E, Rzepa HS, Wu JL, Schleyer PV

*Verification of stereospecific dyotropic racemisation of enantiopure D and L-1,2-dibromo-1,2-diphenylethane in non-polar media*. Chemical Communications (Camb), 30/07/2012, 48, 8943–8945

Murray-Rust P, Rzepa HS

*Semantic physical science*. Journal of Cheminformatics, 03/08/2012, 4 (1), 14

Shaik S, Danovich D, Wu W, Su P, Rzepa HS, Hiberty PC

*Quadruple bonding in C2 and analogous eight-valence electron species*. Nature Chemistry, 01/01/2012, 4, 195–200

Abersfelder K, Russell A, Rzepa HS, White AJ, Haycock PR, Scheschkewitz D

*Contraction and expansion of the silicon scaffold of stable Si6R6 isomers*. Nature Chemistry, 01/01/2012, 4, 195–200

*Pressure and p-jump X-ray studies of lipids and surfactants: together with Professor Richard Templer and Dr Oscar Ces, millisecond pressure-jump apparatus for Diamond synchrotron beamline I22 is being developed with a Facility Development Grant from STFC. This will allow the kinetics and mechanisms of phase transitions in a wide range of soft matter systems (lipids, DNA, liquid crystals, proteins) to be studied. Microsecond p-jump X-ray apparatus is planned as a further future development.*

Thermotropic and lyotropic liquid crystals: with Dr Paul Low and colleagues at Durham University, photoluminescent liquid crystals, which have potential applications in polymeric sheet polarisers, are being studied. This work was featured on the cover of the February 2008 issue of Liquid Crystals. Columnar liquid-crystalline phases formed by zinc porphyrin-based discotic liquid crystals are being investigated together with Gokhan Yahioğlu. In collaboration with the group of Professor Duncan Bruce at York University, the use of a ruthenium-based surfactant for liquid crystal templating of a mesoporous catalyst has been demonstrated.

Lipid microbubbles for ultrasound imaging: together with clinical and non-clinical colleagues, targeted lipid microbubbles for detection of inflammation in myocarditis using ultrasound imaging are under development. New EPSRC funding for this work was announced in December 2008. With Dr Fernando Bresme, molecular dynamics simulations of lipid microbubbles and lipid monolayers are being combined with experimental studies.

**2012 Publications**

Shaw KP, Brooks NI, Clarke JA, Ces O, Seddon JM, Law RV

*Pressure – temperature phase behaviour of natural sphingomyelin extracts*. Soft Matter, 01/01/2012, 8, 1070–1078

Cook AG, Wardell JL, Brooks NJ, Seddon JM, Martinez-Felipe A, Imrie CT

*Non-symmetric liquid crystal dimer containing a carbohydrate-based moiety*. Carbohydrate Research, 01/08/2012, 360, 79–83


*Hydrostatic Pressure Effects on the Lamellar to Gyroid Cubic Phase Transition of Monolinolein at Limited Hydration*. Langmuir, 01/08/2012, 28, 13018–13024


*Engineering de Novo Membrane-Mediated Protein-Protein Communication Networks*. Journal of the American Chemical Society, 26/03/2012, 134, 5746–5749

Sennoga CA, Yeh JS, Alter J, Stride E, Nihoyannopoulos P, Seddon JM, Haskard DO, Hajnal JV, Tang MX, Eckersley RJ

*Evaluation of methods for sizing and counting of ultrasound contrast agents*. Ultrasound in Medicine & Biology, 06/03/2012, 38, 834–845

Tyler, Ali, Law, RV, Seddon, JM


**Professor John Seddon (CP)**

Research is focussed on experimental studies by X-ray and neutron diffraction, optical and electron microscopy, calorimetry, and solid-state NMR of the structure and dynamics of liquid crystalline systems, from lipid model membranes and surfactants, to thermotropic liquid crystals and block copolymers. Applications ranging from templating of mesoporous catalysts, to lipid microbubbles for ultrasound imaging, are also under investigation. During 2008 his EPSRC Platform Grant (jointly with Professor Richard Templer, Drs Rob Law and Oscar Ces) was successfully renewed for a further five years (from February 2009).

DNA-DNA interactions, recognition and assembly: together with Professor Alexei Kornyshev and Dr Geoff Baldwin (Molecular Biosciences), the liquid-crystalline properties of cholesteryl DNA, and the role of homology in DNA-DNA interactions and phase separation, are under investigation. This work has been featured in the following: *Paired pairs*, Research Highlights, *Nature* 451, February 2008, page: 609; *DNA’s self-regard*, Editor’s Choice, *Science*, 319, 15 February 2008, page: 879; *Twin strands of DNA seek each out*, New Scientist Online, 28 January 2008


Lipid membrane microdomains: with Dr Rob Law and Professor Tony Magee (NHIL) the structure and properties of cholesterol-containing model membrane systems are being studied, with a view to their possible roles in various biological functions.
The group focuses on the synthesis and applications of high aspect nanomaterials, particularly carbon nanotubes, but including systems based on titania, zinc oxide, graphene, and layered double hydroxides.

**Professor Milo Shaffer**  
**NMD**  
**Nanostructured hierarchical assemblies and composites Group**

The group focuses on the synthesis and applications of high aspect nanomaterials, particularly carbon nanotubes, but including systems based on titania, zinc oxide, graphene, and layered double hydroxides.

**AREAS OF CURRENT RESEARCH INCLUDE:**

- **Synthesis of carbon and inorganic nanotubes/nanorods, including *in situ* within polymer matrices.**
- **Surface modification and assembly of nanotubes/nanorods for composites, electrodes (capacitors, photovoltaics, fuel cells), and catalyst supports.**
- **(Fine structured) carbon nanotube composites, including foams, and particularly hybrid systems with conventional carbon fibres.**

The last century of materials chemistry has proven the enormous value to society of controlling both the composition and structural arrangement of solid matter. Recently, the potential value of developing nanomaterials systems has been recognised, and has become a major focus of research activity. However, the real opportunity will ultimately derive not from controlling either the nano or the micro regime alone, but integrating the design of the material at every length scale. As yet, we only intentionally tackle one or two rungs on the ladder, but there are five orders of magnitude between a polymer molecule and a human hair; to readapt Feynman, “there is plenty of room in the middle”. Nature already highlights the value of this approach, and although we lack her dexterity, we can use a wider range of chemistry that is not necessarily compatible with physiological conditions. To access this region, we must continue to improve the fundamental synthesis of well-defined building blocks and develop new methods for their assembly.

Carbon nanotubes have provoked enormous interest in their fundamental behaviour and a wide variety of potential applications. They have the greatest strength, thermal conductivity, and electrical current capacity of any substance, and may be metallic or semiconducting depending critically on their chirality. So far, single-wall nanotubes have been used to make the world’s smallest room temperature transistors and the most sensitive (bio-)electronic sensors. However, these applications require the selection of individual tubes with specific electronic character. Unfortunately, nanotubes are always synthesised as a more or less random mixture, including metals and semiconductors. The group has developed new, potentially large volume, strategies to separate and functionalise individual single wall nanotubes, and to assemble them into higher order structures. These new scalable approaches have been recently licensed to a major international manufacturer, and may yet prove to have additional benefits as a means of single-wall nanotube chemical modification. As an alternative, the group has already developed new, scalable gas phase approaches to produce large volumes of chemically-modified multi-wall carbon nanotubes with a minimum of waste; in principle, the method can be adapted to existing equipment for tonne-scale production of nanotubes. The resulting surface chemistry is difficult to study in detail, but by adapting Inverse Gas Chromatography to the requirements of nanoscale structures, surface and specific absorption energies, isotherms/Henry coefficients, and donor–acceptor numbers can all be determined. In further work, on nanotube synthesis, the group grows nanotubes onto conventional micron-sized fibres to create hierarchical structures suitable for both structural and multi-functional composites.

Inorganic nanorods and nanotubes offer an even wider range of functional properties and potential applications. Recent work in the group has produced new types of pure phosphorus and arsenic nanorods that shed light on fundamental questions of allotropy. Work on zinc oxide focuses on the production of nanoreinforcements directly *in situ* within cross-linking engineering resins and conducting polymers for photovoltaic devices. New layered double hydroxides and other compound nanoparticles offer promise as (supported) catalysts. As synthetic methods produce ever more reliable materials, the next challenge is to assemble more complex, hierarchical structures.

The group focuses on building new nano- and meso-structures in reasonably large volumes that are relevant to applications in photovoltaics, electrochemical devices, tissue scaffolds, and composites. It is highly interdisciplinary, collaborating with colleagues both in Chemistry, and in Chemical Engineering, Physics, Materials, Aeronautics, and Medicine.

**2012 Publications**

Orchard KL, Shaffer MSP, Williams CK  
*Organometallic Route to Surface-Modified ZnO Nanoparticles Suitable for In Situ Nanocomposite Synthesis: Bound Carboxylate Stoichiometry Controls Particle Size or Surface Coverage*  
*Chemistry of Materials*, 10/07/2012, 24, 2443–2448

Menzel R, Bismarck A, Shaffer MSP  
*Deconvolution of the structural and chemical surface properties of carbon nanotubes by inverse gas chromatography*  
*Carbon*, 01/08/2012, 50, 3416–3421

Garcia-Gallastegui A, Iruretagoyena D, Gouvea V, Mokhtar M, Asiri AM, Basahel SN, Al-Thabaiti SA, Alyoubi AO, Chadwick D, Shaffer MSP  
*Graphene Oxide as Support for Layered Double Hydroxides: Enhancing the CO₂ Adsorption Capacity*  
*Chemistry of Materials*, 11/12/2012, 24, 4531–4539

Hodge SA, Bayazit MK, Coleman KS, Shaffer MS  
*Unweaving the rainbow: a review of the relationship between single-walled carbon nanotube molecular structures and their chemical reactivity*  
*Chemical Society Reviews*, 19/04/2012, 41, 4409–4429

Milner EM, Skipper NT, Howard CA, Shaffer MS, Buckley DJ, Rahnejat KA, Cullen PL, Heenan RK, Lindner P, Schweins R  
*Structure and morphology of charged graphene platelets in solution by small-angle neutron scattering*  
*Journal of the American Chemical Society*, 14/05/2012, 134, 8302–8305
Cho J, Boccaccini AR, Shaffer MSP
The influence of reagent stoichiometry on the yield and aspect ratio of acid-oxidised injection CVD-grown multi-walled carbon nanotubes
Carbon, 01/09/2012, 50, 3967–3976

Cunningham G, Lotya M, Cucinotta CS, Sanvito S, Bergin SD, Menzel R, Shaffer MS, Coleman IN
Solvent exfoliation of transition metal dichalcogenides: dispersibility of exfoliated nanosheets varies only weakly between compounds
ACS Nano, 06/03/2012, 6, 3468–3480

Layered Double Hydroxide supported on Multi-wall Carbon Nanotubes: preparation and CO₂ sorption characteristics
Journal of Material Chemistry, 20/04/2012, 22, 13932

Professor Alan Spivey (Synthesis)
The Spivey group is engaged in the development of new synthetic concepts and methods and the demonstration of their utility by application to the synthesis of bioactive natural products and of signalling molecules and imaging agents in biological systems.

CURRENT INTERESTS INCLUDE:
Development of New Synthetic Methodology
4-DMAP-based chiral nucleophilic organocatalysts – We are currently developing alcohol and amine acylative/sulfonylative kinetic resolution and asymmetric desymmetrisation procedures catalysed by axially chiral pyridines and pyridine-N-oxides, e.g.

Ge-based phase-tagged synthesis – We are interested in exploiting some unique properties of germanium for organic synthesis. Specifically, we are developing iterative phase-tagged approaches for the preparation of oligomeric organic semiconductors for potential applications in plastic electronic devices. We are also using arylgermanes for isotopic labeling for Positron Emission Tomography (PET) and for pharmaceutical/agrochemical library preparation, e.g.

Total Synthesis of Bioactive Natural Products
Celastraceae sesquiterpenoids – We are engaged in the total asymmetric synthesis of euonyminol, evonic acid, iso-evonic acid which comprise key components of various ANTI-HIV natural products:

Amaryllidaceae alkaloids – We have developed an efficient synthesis of clivonine which exploits a biomimetic interconversion of the lycorine → lycorenine ring systems:

Aspergillus sp. fungal metabolites – We are developing a synthesis of aspercyclide A which is the only known natural product antagonist of an important protein-protein interaction in various human allergic conditions including asthma:

Biological Chemistry – Signal Transduction
Antagonists of the human IgE-FcERI protein-protein interaction – We have a collaboration with Robin Leatherbarrow (Department of Chemistry, Imperial), Brian Sutton and Andrew Beavil (Structural Biology, King’s College London) developing peptide-based antagonists of the above-mentioned protein-protein interaction:

Small molecule regulators of LRH-1 – We have a collaboration with Simak Ali (Oncology, Hammersmith Hospital, Imperial) using in silico and screening techniques to develop antagonists/inverse agonists of the interaction of various coactivator proteins with certain nuclear receptors as an approach to the discovery of new cancer therapeutics:

Development of ⁴¹F labelled HER-1 & HER-1 receptor imaging agents for PET – We have a collaboration with Eric Aboayge (Oncology, Hammersmith Hospital, Imperial) developing methods for ⁴¹F labeling of certain heterocyclic compounds for imaging of breast cancers:
**2012 Publications**

Larionov E, Mahesh M, Spivey AC, Wei Y, Zipse H

Theoretical Prediction of Selectivity in Kinetic Resolution of Secondary Alcohols Catalyzed by Chiral DMAP Derivatives

*Journal of the American Chemical Society*, 06/06/2012, 134, 9390–9399

Warren SA, Stokes S, Frampton CS, White AJ, Spivey AC

Synthesis of anti and syn hydroxy-iso-evoninic acids

*Organic Biomolecular Chemistry*, 17/05/2012, 10, 4685–4688

Offermann DA, McKendrick JE, Sejberg JJ, Mo B, Holdom MD, Helm BA, Leatherbarrow RJ, Beavil AJ, Sutton BJ, Spivey AC

Synthesis and incorporation into cyclic peptides of tolan amino acids and their hydrogenated congeners: construction of an array of A-B-loop mimetics of the Cε3 domain of human IgE

*Journal of Organic Chemistry*, 07/03/2012, 77, 3197–3214


Copper-free click—a promising tool for pre-targeted PET imaging

*Chemical Communications*, 25/01/2012, 991–993

**Dr Joachim H G Steinke (CB)**

Functional, Structural and Supramolecular Polymeric Materials: Dr Steinke's group develops multifunctional polymeric materials for a number of applications. Reducible polycationic polymers have been shown to be superior polymeric vectors for DNA transfection when compared to the current polymer standard PEI, retaining transfection efficiency (in mice) while cytotoxicity has been reduced to background levels (collaboration with M. Thanou and colleagues at King's College London). Gels, networks of polymer chains connected chemically, are of interest for drug delivery, oil recovery and to accelerate drug discovery. In the latter case the development of novel polymer support has continued with new gels as polymer supports which are more universally applicable to automated drug synthesis. In collaboration with Professors Kang Li, Alexander Bismark and Andrew Livingston (all from the Department of Chemical Engineering) new hollow fibre membranes were developed based on polyaniline to the point that they present a commercially viable means of using nanofiltration as method of purification in chemical synthesis. The addition of crosslinking molecules during membrane formation produced chemically stable membranes exhibiting good flux even in polar aprotic solvents such as DMF which provides new opportunities to substitute classical purification processes with the much less energy intensive nanofiltration approach. Synthesis and processing of conjugated polymers, polymer dielectrics and metal inks feature in the collaboration with Alasdair Campbell, Donal Bradley et al. (Department of Physics, Figure 1). The design of a unique multi-layer gravure printing process for organic transistors demonstrates a technology which is amenable to high throughput mass production on flexible substrates in a continuous roll-to-roll (R2R) process. The development of new approaches for ‘greener’ production of porous membranes for Li ion batteries on the basis of high internal phase emulsions is a further activity in the area of advanced materials synthesis for advanced manufacturing (jointly with Alexander Bismark (Department of Chemical Engineering. Figure 2).

**Dr Ed Tate (CB)**

Dr Ed Tate’s research focuses on the development and application of chemical approaches to understand and manipulate living systems. The Tate group is currently undertaking research projects in three main areas:

**Chemical proteomics**

Current research in this area focuses on techniques to probe the role of enzymes in live cells and in vivo (i.e. in live animals). They are developing new methods for high-throughput proteomic analysis of post-translationally modified (PTM) proteins, and for the identification of potential drug targets in antibiotic-resistant infection, developing world disease and cancer.

**Medicinal chemistry**

The development of novel anti-malarial, antibiotic and anticancer agents that target enzymes involved in PTM. The group is also working on developing small-molecule inhibitors of protein-protein interactions involved in bacterial transcription and the invasion of red blood cells by the malaria parasite, with important applications as chemical genetic tools and as potential drug candidates.

**Organic synthesis**

Synthetic organic chemistry is the key enabling tool for research in the Tate group, and they are actively engaged in the development and application of synthetic methodology. They have recently made advances in the areas of cascade cyclisation for bioactive and natural product total synthesis, chemical reactions for engineering biological systems, and the generation and screening of large combinatorial libraries.
Professor Richard Templer

Professor Richard Templer holds the Hofmann Chair in Chemistry. He stood down from his role as Director of the Chemical Biology Doctoral Training Centre to become the Director of Climate-KIC UK, the Head of Education for Climate-KIC and Director of Innovation at the Grantham Institute for Climate Change. Climate-KIC is a pan-European initiative, funded by the European Institute for Innovation and Technology that is designed to catalyse climate change innovation. Professor Templer was part of the bid team that won the seven year contract to work on research, innovation and education in this area and then moved into setting up and leading parts of the programme. Further information on the Climate-KIC can be found at www.climate-kic.org.

Professor Templer's personal research is focussed on two related areas: examining the effects of elastic stresses in lipid membranes on the behaviour of membrane associated proteins and measuring and modelling the energetics and dynamics of transitions between the liquid crystals that form when lipids are mixed with water. Starting in 2010 he has been working with his colleagues, Professor Seddon and Drs Ces, Law and Barter on the development of simple artificial cells that draws on this research.

This year saw Professor Templer and his colleagues publish papers on the molecular factors which stabilise the sponge-like bicontinuous cubic phases. This has particular relevance to the engineering of these nanometre-scale structures for technological purposes. A number of papers were also published on the state of the art in research of the effects of pressure on lyotropic phases and the groups’ development of an automated pressure jump system for the Diamond synchrotron.

The year saw the graduation of three of Professor Templer’s PhD students, Drs Knott, Tang and Casey. Dr Annela Seddon a Research Fellow in the group moved on to a Lectureship at Bristol University, Dr Gemma Shearman a long standing Research Assistant in the group joined DSTL, whilst former students Dr Xavier Mulet and Charlotte Conn were awarded permanent scientific posts at the CSIRO.

Professor Templer also organised an international conference at Chatham House in April to look at key issues surrounding the development of biofuels. He has been editing a special issue of the Royal Society’s Journal Interface that covers the findings of this workshop. His interest in biofuels and related biorenewable technologies have led to a number of international Advisory and Board roles in Brazil (CTBE and BIOEN) and in the Netherlands (BE-BASIC and the Kuyver Centre). He also helped the RAC to organise a new facet of the Brighton Rally in which a rally of low emission vehicles occurred.

Professor Richard Templer

CB

2012 Publications

Furse S, Brooks NJ, Seddon AM, Woscholski R, Templer RH, Tate EW, Gaffney PRJ, Ces O Lipid membrane curvature induced by distearoyl phosphatidylinositol 4-phosphate Soft Matter, 01/01/2012, 8, 3090–3093

Bradshaw RT, Aronica PGA, Tate EW, Leatherbarrow RJ, Gould IR Mutational Locally Enhanced Sampling (MULES) for quantitative prediction of the effects of mutations at protein-protein interfaces Chemical Science, 01/01/2012, 3, 1503–1511

Heal WP, Wright MH, Thinin E, Tate EW Multifunctional protein labeling via enzymatic N-terminal tagging and elaboration by click chemistry Nature Protocols, 01/01/2012, 7, 105–117

Broncel M, Serwa RA, Tate EW A new chemical handle for protein AMPylation at the host-pathogen interface ChemBioChem, 02/01/2012, 13, 183–185


Thinin E, Mann D, Tate EW Targeting N-myristoyl transferase-1 in cancer using peptide microarrays Journal of Peptide Science, 01/09/2012, 18, 575

Price HP, Hodgkinson MR, Wright MH, Tate EW, Smith BA, Carrington M, Stark M, Smith DF A role for the vesicle-associated tubulin binding protein ARL6 (BBS3) in flagellum extension in Trypanosoma brucei Biochim Biophys Acta, 15/05/2012, 1823, 1178–1191

2012 Publications


Metal complexes provide an ideal platform for the development of small molecules that can selectively interact with the active site of enzymes and, in doing so, inhibit their activity. This is due to the great structural flexibility and ease of synthesis of this type of compound. They have particular interest in selectively inhibiting a group of phosphatases with important roles in cell signalling. To this aim, the group is currently investigating the use of target-based synthetic approaches where the phosphatase is exposed to a dynamic combinatorial library (DCL) of compounds with the aim of ‘selecting’ the best possible inhibitor.

**Interaction of small metal complexes with DNA**

DNA can adopt different structures besides its canonical right-handed double helix. Some of these structures can be favoured by interaction with small molecules (such as metal complexes). The group has particular interest in the formation of quadruply-stranded DNA induced by the presence of planar metal complexes. This could have important implications in the development of novel anticancer drugs.

**Development of new probes for molecular imaging**

The magnetic and optical properties of metals, combined with the recognition properties of selected organic ligands, are ideal to design sensitive and selective probes for bio-imaging. Based on this approach, group members are currently developing probes for Magnetic Resonance Imaging (MRI), Positron Emission Tomography (PET) and Optical Imaging.

**Inhibition of phosphatases by small metal complexes**

Metal complexes provide an ideal platform for the development of small molecules that can selectively interact with the active site of enzymes and, in doing so, inhibit their activity. This is due to the great structural flexibility and ease of synthesis of this type of compound. They have particular interest in selectively inhibiting a group of phosphatases with important roles in cell signalling. To this aim, the group is currently investigating the use of target-guided synthetic approaches where the phosphatase is exposed to a dynamic combinatorial library (DCL) of compounds with the aim of ‘selecting’ the best possible inhibitor.

Their interest is centred in developing new receptors (based on metal complexes and hydrogen bonding ligands) for the selective molecular-recognition of specific analytes. They have particular interest in using these species for sensing and recognition of anions with important biomedical roles (e.g. phosphorylated species, chlorides) or environmental impact (e.g. cyanides). They are also interested in understanding and using non-covalent interactions between anionic species and transition metal complexes (with hydrogen-bonding ligands) for the synthesis of complex supramolecular assemblies.

### 2012 Publications

  A cyclometallated platinum complex as a selective optical switch for quadruplex DNA Chemistry, 14/12/2012, 18, 16277–16282

- **Jimeno C, Christmann U, Escudero-Adan EC, Vilar R, Pericas MA**
  Studies on the Amination of Aryl Chlorides with a Mononivalent Palladium Catalyst: Kinetic Evidence for a Cooperative Mechanism Chemistry, 01/12/2012, 18, 16510–16516

- **Gong X, Miller PW, Gee AD, Long NJ, deMello AJ, Vilar R**
  Gas–Liquid Segmented Flow Microfluidics for Screening Pd-Catalyzed Carbonylation Reactions Chemistry, 01/01/2012, 18, 2768–2772

- **Campbell NH, Abd Karim NH, Parkinson GN, Gunaratnam M, Petrucci V, Todd AK, Vilar R, Neidle S**
  Molecular Basis of Structure-Activity Relationships between Salphen Metal Complexes and Human Telomeric DNA Quadruplexes Journal of Medicinal Chemistry, 12/01/2012, 55, 209–222

- **Suntharalingam K, Hunt DJ, Duarte AA, White AJ, Mann DJ, Vilar R**
  A tri-copper(i) complex displaying DNA-cleaving properties and antiproliferative activity against cancer cells Chemistry – A European Journal, 11/10/2012, 18, 15133–15141

- **Tate CW, Gee AD, Vilar R, White AJP, Long NJ**
  Reversible carbon monoxide binding at copper(i) P-S-X (X=N, O) coordination polymers Journal of Organometallic Chemistry, 15/09/2012, 715, 39–42

- **Herranz F, Schmidt-Weber CB, Shamiji MH, Nakrus A, Ruiz-Cabello J, Vilar R**
  Superparamagnetic iron oxide nanoparticles conjugated to a grass pollen allergen and an optical probe Contrast Media Mol Imaging, 01/07/2012, 7, 435–439

- **Martí-Centelles V, Burguete MI, Galindo F, Izquierdo MA, Kumar DK, White AJP, Luis SV, Vilar R**
  Fluorescent Acridine-Based Receptors for H2PO4−: Kinetic Evidence for a Cooperative Mechanism Studies on the Amination of Aryl Chlorides with a Mononivalent Palladium Catalyst: Kinetic Evidence for a Cooperative Mechanism Journal of Organometallic Chemistry, 14/12/2012, 18, 16277–16282

- **Suntharalingam K, Łęczkowska A, Vilar R**
  Superparamagnetic iron oxide nanoparticles conjugated to a grass pollen allergen and an optical probe Contrast Media Mol Imaging, 01/07/2012, 7, 435–439

### Professor Tom Welton (CAM)

Green chemistry; sustainable chemistry; synthesis and catalysis in ionic liquids; kinetics, physical organic chemistry.

Sustainable or Green Chemistry aims to make the chemicals, and related, industries both environmentally and economically sustainable. It encompasses a range of activities, such as making biodegradable products, sourcing chemicals from renewable resources and/or making chemical processes more efficient in energy and less wasteful in materials. Since solvents are
by far the largest amount of any materials used by the chemicals industries (ca. 20 billion kg per year) and they are usually volatile organic compounds that can be environmentally damaging, they are important targets for anyone interested in improving the sustainability of those industries.

Professor Tom Welton is interested in replacing environmentally damaging solvents with more sustainable ones. He is also using these new solvents to improve chemical processes. He has worked with ionic liquids throughout his research career. Recently, interest from both academic and commercial chemists in these has increased dramatically. His work has made a significant contribution to this change in attitudes. He also works with other solvents, e.g. siloxanes, PEG’s and solvents from renewable resources, all with a view to the development of sustainable solvent technologies. His research covers a broad range of the chemical sciences and he has been the author of papers in all three of the traditional branches of the subject (Inorganic, Organic and Physical). He is particularly interested in clean synthesis and catalysis.

The central academic aim of his research is to understand the role that the immediate chemical environments in which reacting species find themselves influence the reaction process. He also aims to use this understanding to provide more effective chemical processes by the matching of the reaction with the optimum reaction environment. The principal foci of his investigations are the reactions themselves and how they change in rate, product distributions etc. His group correlate their synthetic results with calculated values (e.g. gas phase acidities) and physical measurements (e.g. the spectra of probe dye molecules).

IMPORTANT ADVANCES THAT HIS GROUP HAVE MADE IN THE PAST YEAR HAVE INCLUDED:

• Discovering the first unique ionic liquid effect on a chemical reaction
• The first successful design of an ionic liquid to be the best solvent for a specific reaction
• Understanding how ionic liquids interact with nucleophiles to change their reactivity

2012 Publications

Niedermeyer H, Hallett JP; Villar-Garcia IJ, Hunt PA, Welton T

MIXTURES OF IONIC LIQUIDS

Chemical Society Reviews, 13/08/2012, 41, 7780–7802

Bulut S, Ab Rani MA, Welton T, Lickiss PD, Krossing I

PREPARATION OF [Al(THF)4]-BASED IONIC LIQUIDS WITH SILANOANE-FUNCTIONALIZED CATIONS AND THEIR PHYSICAL PROPERTIES IN COMPARISON WITH THEIR [TF2N]-ANALOGUES

ChemPhysChem, 12/03/2012, 13, 1802–1805

Skarmoutsos I, Delli D, Matthews RP; Welton T, Hunt PA

HYDROGEN BONDING IN 1-BUTYL-AND 1-ETHYL-3-METHYLLIMIDAZOLOIUM CHLORIDE IONIC LIQUIDS

Journal of Physical Chemistry B, 16/04/2012, 116 (16), 4921–4933

Brandt A, Erickson JK, Hallett JP, Murphy RJ, Potthast A, Ray MJ, Rosenau T, Schrem M, Welton T

SOAPING OF PINE WOOD CHIPS WITH IONIC LIQUIDS FOR REDUCED ENERGY INPUT DURING GRINDING

Green Chemistry, 01/01/2012, 14, 1079–1085

Dr Paul Wilde (CP)

Dr Paul Wilde’s research is based in electrochemistry and has two main components: the use of non-linear optical spectroscopy (specifically Second Harmonic Generation or SHG) to examine the growth of oxide films (particularly those with multilayer structures) on metal surfaces and the surface chemistry of semiconductors, and the use of self-assembled monolayers to modify the reactivities of metal electrodes and metal nanoparticles.

In SHG, a laser beam with a frequency ω is shone at an electrode but the reflected beam with a frequency of 2ω is detected. This second harmonic signal is sensitive to interfacial properties and particularly to changes in interfacial chemistry and bonding. Together with Dr Alan Taylor we have pioneered the use of SHG to examine oxide growth under potential control, especially where the metal oxide forms a multilayer or duplex structure with one oxide on top of another.

We have demonstrated that analysis of the SHG signal provides information about the chemical and electronic properties of the oxides formed (some of the oxides produced are semi-conductors) together with insight into the mechanism of oxide formation and reduction (many interesting questions still remain unanswered in this area). In the other research theme, electrochemical methods are being employed to prepare self assembled monolayers of alkane thiols (RSH, where R is an alkyl group) on electrode surfaces and then partially remove the layer before depositing a second, different thiol.

This method allows the controlled formation of surfaces with patterned, mixed chemical or physical properties and these surfaces are of interest in areas such as sensing for multiple analytes using one surface because different sensing agents (enzymes, antibodies, complexing agents) can be attached to different parts of the surface.

Finally metal nanoparticles are grown using simple reduction of metal salts at electrodes in the presence of selected alkane thiols, a process that leads to the formation of particles with a preferred orientation of crystalline faces (crystal faces have different catalytic abilities) and therefore allows nanoparticles with enhanced catalytic activity to be prepared with ease. This process is being studied in detail in order to confer improved control and hence to allow reproducible preparation of catalysts with enhanced properties.

Professor Charlotte Williams (NMD)

Professor Williams’ research interests lie in the areas of catalysis, polymer and materials chemistry. In particular the preparation and study of new polymerisation catalysts is a significant research interest. In this context, the group have interests in the coordination chemistry of main group and transition metal complexes, which have subsequently been used as highly active polymerisation catalysts. She has particular expertise in ring-opening polymerisation reactions, for example of lactones and the sequential copolymerisation of carbon dioxide and
heterocycles. These polymerisations enable the controlled synthesis of polyesters, polycarbonates, polycarbamates, etc. In the areas of polymerisation catalysis, the Williams group have recently published a series of new catalysts which show excellent activities and good control for the sequential copolymerisation of epoxides and carbon dioxide. The catalysts are particularly unusual because they operate under mild conditions (including at just 1 atm pressure of CO₂) and are tolerant. The catalysts are dinuclear metal complexes, including of Zn(II), Co(II/III) and Fe(II) and show very high activities and long life-times. The di-Zn(II) complex was the first competent catalyst to work at 1 atm pressure. Currently, research is focussed on carrying out structure-activity studies on the new catalysts, studying the copolymerisation kinetics and elucidating the reaction mechanism. In the area of lactone (lactide) ring-opening polymerisation, the Williams group have reported and studied a series of yttrium initiators which show very high rates of polymerisation. A full structure-activity study was carried out, and in combination with kinetic studies, an improved understanding of the controlling factors in the mechanism was obtained: it is likely that for this class of catalysts insertion reactions dominate. The group also discovered that the polymer tacticity was controlled by the nuclearity of the initiator: highly heterotactic PLA could be produced. Currently, the group continue to research new initiators for lactide ring opening polymerisation, focussing on metal complexes of Group 3 and 13 and on the preparation of isotactic and stereocomplex PLA. As part of a cross-College team, the group are also investigating the activation and reduction of carbon dioxide using both well-defined inorganic compounds and metal/metal oxide nanoparticles as catalysts. The project is being led by Professor Williams and addresses various different approaches including photochemical CO₂ reduction (Professor Durrant), electrochemical and thermochemical reduction (Dr Klaus Hellgardt, Department of Chemical Engineering) and thermochemical reduction (Dr Klaus Hellgardt, Department of Chemical Engineering and Professor Shaffer).

Professor Williams has expertise in the preparation and properties of degradable polymers, including polylactide, other aliphatic polyesters and the development of new biocompatible and degradable materials. Recently, the group have reported the preparation of a lactone derived from D-glucose in high yield. The lactone synthesis is achieved in two steps and in high yield, scale-up experiments are on-going. This new carbohydrate derived lactone can be copolymerised with lactide to yield random copolymers. The degradation of PLA can be controlled by varying the quantity of the carbohydrate lactone. Currently, the group are investigating the preparation of a range of new bio-derived, degradable polymers and also characterising their thermo-mechanical properties (with Professor Bismarck, Department of Chemical Engineering). The application of the new polymers and copolymers in tissue regeneration and controlled release is being investigated in collaboration with Professor Molly Stevens (Department of Materials).

The Williams group also investigate the synthesis and properties of new conjugated polymers and organometallic complexes. In particular, a series of iridium-conjugated polymer complexes have been prepared and used as the red emitting layer in polymer light emitting diodes. The structure-activity study revealed in the influence of both the type of substituent and its regiochemistry on the photophysical properties. These conjugated polymer complexes have also been important tools in the study of polymer photovoltaics. This work has been in collaboration with Professor Richard Friend, Cavendish laboratory, Cambridge. The preparation of ZnO nanoparticles and nanocomposites (in epoxy resins) is being actively researched by the Williams group. The ZnO is prepared via the hydrolysis of organometallic zinc complexes which has proved to be an efficient and rapid means to prepare well defined ZnO nanoparticles. This has also led to the preparation and study of various organometallic zinc complexes, including alkyl zinc carboxylate complexes, as precursors for ZnO synthesis. This work is in collaboration with Professor Milo Shaffer.

**Prize**

*Bio-environmental Polymer Society Outstanding Young Scientist Award for 2011.*

**2012 Publications**

Kember MR, Williams CK *Efficient magnesium catalysts for the copolymerization of epoxides and CO₂ using water to synthesize polycarbonate polyols* Journal of the American Chemical Society, 26/09/2012, 134, 15676–15679


Lee K-Y, Tang M, Williams CK, Bismarck A *Carbohydrate derived copoly(lactide) as the compatibilizer for bacterial cellulose reinforced polylactide nanocomposites* Composites Science and Technology, 17/09/2012, 72, 1646–1650


Kember MR, Copley J, Buchard A, Williams CK *Triblock copolymers from lactide and telechelic poly(cyclohexene carbonate)* Polymer Chemistry, 01/01/2012, 3, 1196–1201


Orchard KL, Shaffer MSP, Williams CK *Organometallic Route to Surface-Modified ZnO Nanoparticles Suitable for In Situ Nanocomposite Synthesis: Bound Carboxylate Stoichiometry Controls Particle Size or Surface Coverage* Chemistry of Materials, 10/07/2012, 24, 2443–2448


Kember MR, Jutz F, Buchard A, White AJP, Williams CK *Bi-cobalt(II) catalysts for the copolymerisation of CO, and cyclohexene oxide: support for a dinuclear mechanism?* Chemical Science, 01/01/2012, 3, 1245–1255
determined the atomic structure of the closed form of this yeast CCT-actin complex by X-ray crystallography. The structural studies all point to a remarkably asymmetrical machine with the features required to support a sequential allosteric folding mechanism able to bind specifically and anneal the non-native actin polypeptide. We believe that the final outcome of the CCT-dependent actin folding mechanism is to produce a protein spring whereby the actin monomer is able to reversibly re-explore the folding landscape in the structural context of the polymeric F-actin filament.

We have been applying systems biology approaches to discover further activities of CCT in yeast using high-throughput proteomics and transcriptomics. At the Weizmann Institute high-throughput microscopy techniques have been developed, by Dr Maya Schuldiner, which permit the interrogation of thousands of yeast strains in parallel experiments. This year we used this technology with Professor Amnon Horovitz to investigate CCT function. Mutants in yeast CCT were screened and revealed interactions between CCT and Q/N-rich proteins (Nadler-Holly et al, 2012). Q/N-rich proteins are implicated in human protein aggregation conditions such as Alzheimer’s diseases.

We now intend to study the CCT system in humans and the first stage is to construct functional folding assays using purified components. Dr Kodai Machida, University of Hyogo, Japan has purified human CCT and a reconstituted human ribosome translation system. He visited our group at Imperial this year and showed that the pure human CCT is functional in actin folding. This is a promising development.

**Single cell proteomics**

Single molecule counting approaches are not only an essential approach for clinical and pre-clinical science and systems medicine but also for generating precise quantitative data for the mathematization of biology. The holy grail of single cell proteomics is the ability to count, within high dynamic range, the copy numbers, protein-protein interactions and post-translational modifications of many proteins in individual cells using label-free approaches. Here, label-free means that the proteins are not pre-labelled before analysis: for example by using GFP-gene tagging or in vivo chemical labelling technologies. Professor David Klug and I are working to develop robust, high-throughput methods to count, at single molecule sensitivity, proteins found in bodily fluids and in rare cells present in clinical biopsies. Single molecule detection is highly accurate, does not require calibration and the read-out is digital. We have created a multi-disciplinary laboratory environment to implement and to invent the tools and technologies (T&Ts) needed to achieve these ambitious goals. At this stage in the development of this field most of the T&Ts are by no means plug and play and require expertise in engineering (microfluidics), applied optics (total internal reflection fluorescence and optical trapping spectroscopies), mathematics (data analysis and model building), cell biology (cell separation and manipulation), protein chemistry (antibody development) and chemistry (probe use and development). The first prototype device is the MAC chip (Microfluidic Antibody Capture) which has been used to count p53 tumor suppressor proteins at single molecule level in single colorectal cancer cells with 88% accuracy.

**2012 Publications**


Interactions of subunit CCT3 in the yeast chaperonin CCT/TRiC with Q/N-rich proteins revealed by high-throughput microscopy analysis

Proceedings of the National Academy of Sciences USA, 2012, 109, 18833–18838

Goyder MS, Willison KR, Klug DR, de Mello AI, Ces O

Affinity chromatography and capillary electrophoresis for analysis of yeast ribosomal proteins

BMB Rep, 01/04/2012, 45, 233–238

**Professor Keith Willison (CB)**

**Protein folding and CCT**

The cytosolic chaperonin CCT is a 1-MDa multi-subunit protein complex that has an essential, core function in actin protein folding in all eukaryotes. In 2011 we determined the atomic structure of the closed form of this yeast CCT-actin complex by X-ray crystallography. The structural studies all point to a remarkably asymmetrical machine with the features required to support a sequential allosteric folding mechanism able to bind specifically and anneal the non-native actin polypeptide. We believe that the final outcome of the CCT-dependent actin folding mechanism is to produce a protein spring whereby the actin monomer is able to reversibly re-explore the folding landscape in the structural context of the polymeric F-actin filament.

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**Dr James Wilton-Ely (CAM)**

James Wilton-Ely obtained both his BSc and PhD at Imperial, the latter conducted in the group of Professor Tony Hill. His initial research interests were in the field of polydentate ligands with sulfur and nitrogen donors and their role in stabilising vinyl and phosphavylnil ligands created in the coordination sphere. After a year as Fixed-Term Lecturer at Imperial, he departed to work in the very different area of gold thiolate compounds as a von Humboldt Fellow with Professor Hubert Schmidbaur at the Technical University in Munich. In order to also add a knowledge of catalysis and the interface with industry, he returned to the UK to work on cobalt catalysed hydroformylation of long chain alkenes with Professor David Cole-Hamilton at the University of St Andrews. His independent career started back in London at UCL where he was awarded a Ramsay Fellowship and continued his research as FitzJames Fellow in Oxford two years later. In the three and a half years spent at Merton College, he developed new routes to the surface functionalisation of gold nanoparticles, aimed at catalysis and sensing. Among other topics, it is this field that forms the focus of his work at Imperial, where he started a Lectureship in Inorganic Chemistry in January 2009.

The research group works mainly with sulphur-based systems, in particular thiolis and dithiocarbamates to construct new, often multimetallic, materials suitable for applications in fields as diverse as molecular electronics, (bio)sensing and catalysis. Although the systems range in orders of magnitude (monometallic compounds to gold nanoparticles), the key to our work is our broad expertise in synthetic organic, organometallic and coordination chemistry.

**AREAS OF CURRENT INTEREST INCLUDE:**

- Transition metal functionalised gold nanoparticles
- Catalysis supported by sulphur ligands
- Functionalised thiolis for SAM-based nanotechnology applications
- Multimetallic compounds
- Breakdown and catalytic conversion of biomass to platform chemicals

In conjunction with Dr Graeme Hogarth and Dr Katherine Holt at UCL, we have explored the potential of dithiocarbamate ligands to link metal centres together in homo- or heteronuclear systems. The ability to utilise the properties of two or more metals in the same ensemble allows the material to exhibit diverse and...
complementary reactivity within the same system. This can lead to two metals performing catalysis in tandem or the physiological fate of a cytotoxic unit being traceable due to a luminescent metal-based tag. An extension of the methodology we use to achieve this allows the attachment of a metal unit (chosen for its properties) to be immobilised on the surface of gold nanoparticles (see figure 1 below). The large surface area and pre-organised surface arrangement coupled to the marked difference in physical properties give these materials significant benefits over conventional homogeneous or heterogeneous systems in terms of activity, selectivity and recycling of the material. We are in the process of investigating these functionalised nanoparticles using computational methods with Dr Fernando Bresme. This will allow us to improve their design and determine the relative strength of interactions between the surface and the sulphur units attached with a view to constructing mixed surface topographies.

Although dithiocarbamates have proved effective in the tethering of transition metal units to the surface of the nanoparticles, we are also exploring other methods of adding functionality to nanoparticles through straightforward and reliable organic transformations (e.g. click or metathesis chemistry). The incorporation of the innate properties of the metal core of the nanoparticle, such as magnetism, is also under investigation.

In addition to three dimensional gold surfaces, we are also actively engaged in a collaboration with Dr Manfred Buck at the university of St Andrews to design biphenylalkane thiols, which can form large, almost defect-free domains on Au(111) surfaces. Functionalisation of the surface functionality will allow the deposition of metal units, which may ultimately lead to the fabrication of surface features functioning as electronic components.

In 2011, a new area of research was initiated in collaboration with Dr Jason Hallett, directed at the breakdown of biomass and its conversion into platform chemicals. This approach employs metal catalysts in ionic liquids to dissolve the cellulosic component of biomass and convert it catalytically into 5-hydroxymethylfurfural (5-HMF) – a versatile starting point for many chemical building blocks. This approach could provide a non-petrochemical source for many of the fundamental compounds on which the chemical industry depends.

Figure 1

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Dr Rudiger Woscholski (CB)

Lipid mediated signalling in cells is critical for the development and control of many diseases, such as cancer and diabetes. Over the last decade the Woscholski group has been pioneering the validation and application of new chemical intervention tools targeting lipid metabolising enzymes as well as the lipids themselves and their corresponding effectors. Currently we are exploring the chemical space of key proteins in lipid mediated signalling to create specific, potent and cell-permeable modulators in order to elucidate their corresponding cellular function using mammalian and plant systems.

One of our research interests is on cysteine-based phosphatases, such as the tyrosine and inositol phosphatases, which are important modulators of cellular signalling pathways. The loss of function of these phosphatases will often result in severe physiological consequences. For example the inositol phosphatase PTEN counteracts cell growth inducing signals and is thus known as a tumour suppressor. We developed and characterised a specific and potent small molecule inhibitor of PTEN that was subsequently employed to prove that a partial loss of PTEN function causes cancer, whereas the total loss of function will trigger cellular senescence. This observation demonstrated that the inhibition of PTEN function by chemical inhibitors might well be beneficial for cancer therapy. In this context the Woscholski group is currently investigating the underlying biochemical mechanisms of phosphatase enzymology and pharmacology.

Biological protein-based metabolite recognition tools are currently used in research to detect inositol lipids. Another research focus in the Woscholski group is the development and application of small molecule mimetics that have similar characteristics as their biological model proteins. Detection of the phosphoinositide lipid PtdIns(4,5)P2 in cells or in lipid extracts is facilitated by the use of the PH domain of the enzyme phospholipase C. A small molecule mimic of this particular protein domain was recently tested and validated by our research group demonstrating that this chemical intervention tool is capable of lowering the cellular levels of this important lipid. Elevated levels of PtdIns(4,5)P2 are characteristic for Lowe syndrome due to the loss of an inositol phosphatase called OCRL. The PH domain mimetic could therefore be the first step for the development of potential drugs for this X-chromosome linked disorder.

Phosphoinositide signalling is often activating the protein kinase Akt/PKB, which is in turn passing on the signal to other downstream mediators. Chemical intervention tools that affect the activation status of this particular kinase have been developed and are currently validated and applied to identify their

2012 Publications

Synthesis and reactivity of dialkylthiophosphate complexes of ruthenium(II)
RSC Advances, 01/01/2012, 2, 999–1008

Synthesis and catalytic application of palladium imidazol(in)ium-2-dithiocarboxylate complexes
Dalton Transactions, 25/09/2012, 41, 12386–12394

Figure 1
corresponding targets. For example, our group identified small molecule chemicals that activate the kinase Akt, and in doing so mimic the action of growth factors.

**2012 Publications**


*Engineering de novo membrane-mediated protein-protein communication networks*  
Journal of the American Chemical Society, 26/03/2012, 134, 5746–5749


*Osmosensitive changes of carbohydrate metabolism in response to cellulose biosynthesis inhibition*  
Plant Physiology, 15/03/2012, 159, 105 - 117

**Professor Sophia Yaliraki**  
(CB)

**Multiscale dynamics in complex systems: From molecules to systems**

The realisation that there is a molecular basis to biological function, and conversely to loss of function which leads to disease, has prompted a shift in the study of biological and biomedical systems towards an emphasis on the chemical interactions that underpin physiology. Our goal is to develop new mathematical and computational frameworks that can address the molecular basis (and loss) of biological function at different time and length scales.

Our interdisciplinary approach brings together mathematical tools from algebraic geometry, model reduction, graph theory, non-convex optimisation and the theory of stochastic processes in an integrated multi-level methodology. It is fundamentally different from Biomolecular Simulation (potential-determined), Bioinformatics (statics) or Systems Biology (closed loop input-output biological modelling). We have already introduced frameworks that can be applied to a variety of problems in biology and medicine, including applications to: protein engineering and enzyme catalysis, protein aggregation processes associated with disease and infection, molecular imaging (PET), and modelling of gene expression. We are currently pursuing further applications in the design of biomimetic scaffolds for tissue engineering (Artificial Heart Project, Collaboration with the Heart Science Centre at Harefield, The Magdi Yacoub Institute, the Institute of Biomedical Engineering and IMS).

Our theoretical frameworks are equally applicable to the design of nanoscale devices.

We are currently pursuing this in connection with the missing element, the memristor for the fabrication of nanoscale memristive systems.

**TWO SELECTED HIGHLIGHTS INCLUDE:**

**Multiscale partitionings of complex networks**

Networks and graphs provide a useful tool to represent and summarize information about systems in fields as diverse as biology, the social sciences and spanning from engineered and computational systems to economics and financial networks. In such complex networks, it is sometimes helpful to extract meaningful communities or subgroups that are tightly interlinked and act coherently. Finding such communities can provide insights into the structure and functioning of the system and lead to possible simplified descriptions. Recently, we have developed a new method that uses the time-evolution of a process on the network to detect such coherent subgroups. The method allows us to obtain for the first time partitions of the network as a function of time. The introduction of time in this analysis has had an unexpected bonus: it allows us to interpret in a unified framework a series of standard methods that had been introduced ad hoc in the literature over several decades. The method has been applied to the analysis of citation networks, protein structures, web graphs among other systems. The work has received wide attention in different areas of application.

**2012 Publications**


*Acute manipulation of diacylglycerol reveals roles in nuclear envelope assembly & endoplasmic reticulum morphology*  
PloS One, 01/01/2012, 7

Furse S, Brooks NJ, Seddon AM, Woscholski R, Templer RH, Tate EW, Gaffney PRL, Ces O

*Lipid membrane curvature induced by distearoyl phosphatidylinositol 4-phosphate*  
Soft Matter, 01/01/2012, 8, 3090–3093

Mak LH, Knott J, Scott KA, Scott C, Whyte GF, Ye Y, Mann DJ, Ces O, Stivers J, Woscholski R

*Arylstibonic acids are potent and isoform-selective inhibitors of Cdc25a and Cdc25b phosphatases.*  
Bioorg Med Chem, 24/05/2012, 20, 4371–4376
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# Chemistry with Management

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<td>Josh Stephen McNicoll</td>
<td>The production of novel metal-organic frameworks for carbon dioxide capture</td>
<td>Dr Robert Davies</td>
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<tr>
<td>Jenifer Eve Mizen</td>
<td>Fluorogenic click reactions</td>
<td>Dr Ed Tate</td>
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<tr>
<td>Philip Murray</td>
<td>Synthesis of novel derivatives of 1,7-Diaza[5,5]dodecane – a neglected heterocycle</td>
<td>Professor Anthony Barrett</td>
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<tr>
<td>Sadia Rahman</td>
<td>Understanding the regulatory mechanisms controlling photosynthesis; probing rubisco and rubisco active interactions</td>
<td>Dr Laura Barter</td>
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<tr>
<td>Philip Neil Raymond</td>
<td>Lead optimisation of a novel (CdC_2) phosphatase inhibitor</td>
<td>Dr Caroline Low</td>
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<tr>
<td>Ryan Kevin Spence</td>
<td>Improving solid-state dye-sensitized solar cells fabricated from melt processed hole conductors</td>
<td>Dr Brian O’Regan</td>
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<tr>
<td>Laura Claire Stevenson</td>
<td>The carbonylation of polyhydric alcohols</td>
<td>Dr George Britovsek</td>
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<tr>
<td>Rajinder Virdee</td>
<td>Synthesis and characterisation of benzothiophene polymers for organic field effect transistors</td>
<td>Professor Iain McCulloch</td>
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<td>Bamaby Walker</td>
<td>Synthesis of gold nanorods in a microfluidic droplet reactor</td>
<td>Professor John de Mello</td>
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<td><strong>UPPER SECOND</strong></td>
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<tr>
<td>Hiren Bhavsar</td>
<td>Towards a new family of dithiocarbamate-based multimetallic MRI contrast agents</td>
<td>Dr James Wilton-Ely</td>
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<tr>
<td>Sara Cesarec</td>
<td>Fast and efficient reactions of carbon disulfide for positron emission tomography labelling students</td>
<td>Dr Philip Miller</td>
</tr>
<tr>
<td>Marco Antonio Couch</td>
<td>Design, testing and implementation of a synoptic lab project for first year undergraduate students</td>
<td>Dr Andrew McKinley and Dr Laura Patel</td>
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<tr>
<td>Sarah Gates</td>
<td>Activation of inert C-H bonds with monomeric aluminium imide and phosphinidene complexes</td>
<td>Dr Mark Crimmin</td>
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<td>Cosma Enrico Angelo Gottardi</td>
<td>Isolation of regioisomers of coresubstituted perylene diimides and synthesis of derivatives for use as n-type semiconductors in organic photovoltaics and organic field effect transistors</td>
<td>Dr Nicholas Evans</td>
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<tr>
<td>Douglas Hunt</td>
<td>Interaction of mono-, bis- and tri-copper complexes with duplex and quadruplex DNA</td>
<td>Professor Ramon Vilar</td>
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<tr>
<td>Nakai Jirira</td>
<td>Phase behaviour of phosphatidylinositol lipids</td>
<td>Dr Oscar Ces</td>
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<td>Hilary Hiu Lui Kwong</td>
<td>Asymmetric synthesis of chiral N-heteroaryl-substituted beta-amino acids</td>
<td>Dr Mimi Hii</td>
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<tr>
<td>Jonathan Chun Yan Lau</td>
<td>The Synthesis of two novel phthalocyanines</td>
<td>Dr Martin Heeney</td>
</tr>
<tr>
<td>Charlene Frances Lawton</td>
<td>The electrochemical dissolution and deposition of single-walled carbon nanotubes</td>
<td>Professor Milo Shaffer</td>
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<tr>
<td>Fiona Ka Wing Li</td>
<td>Synthesis of a five residue (a)-helix mimic</td>
<td>Professor Alan Spivey</td>
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<tr>
<td>Chia Bai Lin</td>
<td>Electrochemical deposition and characterisation of gold nanoparticles on glassy carbon support</td>
<td>Dr Paul Wilde</td>
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<tr>
<td>Pik Ki Ma</td>
<td>Synthesis of new catalysts for (CO) copolymerisation</td>
<td>Professor Charlotte Williams</td>
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<tr>
<td>Kelsey Chow Mok</td>
<td>Tetradentate internal donors in ziegler-natta catalysts</td>
<td>Dr George Britovsek</td>
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<tr>
<td>Daniel John Brian Morgan</td>
<td>Towards a solid phase synthesis of a library of acrylamides</td>
<td>Professor Alan Armstrong</td>
</tr>
<tr>
<td>Jack William Kyffin Paget</td>
<td>Towards the total synthesis of (Sch) 47554</td>
<td>Professor Anthony Barrett</td>
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<tr>
<td>Madeline Ross</td>
<td>Design and synthesis of a linker for a novel site-directed strategy for drug discovery</td>
<td>Professor Alan Armstrong</td>
</tr>
<tr>
<td>Christopher Kevin Wood</td>
<td>Inorganic nanoparticles as multi-modal MRI probes</td>
<td>Professor Nick Long</td>
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<tr>
<td>LOWER SECOND</td>
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<tr>
<td>Timothy Nicholas Arbabzadah</td>
<td>Core-shell nanoparticles for use in fuel cell catalysis</td>
<td>Dr Tim Albrecht</td>
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<tr>
<td>Signe Liepina</td>
<td>De-aromatising decarboxylative claisen rearrangement reactions</td>
<td>Professor Donald Craig</td>
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<tr>
<td>Thomas Michael Lei Kiat McDevitt</td>
<td>Amine activated utilisation of carbon dioxide as an efficient source of carbon in synthesis</td>
<td>Dr Bao Nguyen</td>
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<tr>
<td>Christine Louise McGee</td>
<td>The palladium catalysed derivatisation of organic azides</td>
<td>Dr Silvia Diez-Gonzalez</td>
</tr>
<tr>
<td>Prima Thakrar</td>
<td>New technologies for single cell biopsies</td>
<td>Dr Oscar Ces</td>
</tr>
<tr>
<td>Jun Yi Xing</td>
<td>The potential of volatile methylsiloxyanes as environmentally benign solvents</td>
<td>Dr Paul Lickiss</td>
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</tbody>
</table>

**Chemistry with Research Abroad**

**FIRST**

<table>
<thead>
<tr>
<th>Name</th>
<th>Project</th>
<th>Supervisor</th>
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<tbody>
<tr>
<td>Saleem Butt</td>
<td>Synthesis of lipophilic iminosugars</td>
<td>Professor Herman Overkleeft</td>
</tr>
<tr>
<td>Joanna Yue Yang Cai</td>
<td>Radical xanthate addition onto alkenes</td>
<td>Professor Samir Zard</td>
</tr>
<tr>
<td>Thomas Edmund Chavas</td>
<td>Optimisation and scope of a gold-catalysed oxidative cyclisation</td>
<td>Professor Fabien Gagosz</td>
</tr>
<tr>
<td>Hamza Giaffar</td>
<td>The facile formylation of organoboron compounds</td>
<td>Professor Pier Giorgio Cozzi</td>
</tr>
<tr>
<td>Emma Oakton</td>
<td>Preparation and characterisation of silica supported Ag nanoparticles through single-site surface species</td>
<td>Professor Christophe Copert</td>
</tr>
<tr>
<td>Peter Swallow</td>
<td>Palladium catalysed carbo-alkynylation of olefins</td>
<td>Professor Jerome Waser</td>
</tr>
<tr>
<td>Holly Yu</td>
<td>Efforts towards the development of an ion-pairing catalyst for the asymmetric total synthesis of malagashamine</td>
<td>Professor Simon Blackey</td>
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**UPPER SECOND**

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<thead>
<tr>
<th>Name</th>
<th>Project</th>
<th>Supervisor</th>
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<tbody>
<tr>
<td>Benjamin Heller</td>
<td>LUV encapsulation of a fluorophore-tagged bioactive peptide</td>
<td>Dr Gerard Chassaing</td>
</tr>
<tr>
<td>Christian Loftus</td>
<td>Quantifying and reducing the self-interaction error of LC functionals in KS-DFT using fractional occupation and IP tuning</td>
<td>Dr David Sherrill</td>
</tr>
<tr>
<td>Hazel Neighbour</td>
<td>Improvement of the in-cellulo activity and localisation of a manganese superoxide dismutase mimic</td>
<td>Professor Clotilde Policar</td>
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<tr>
<td>Ines Rhineberger</td>
<td>Acylphosphane photoinitiators with special reducing properties</td>
<td>Professor/Dr Hansjorg Grutzmacher</td>
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**LOWER SECOND**

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<thead>
<tr>
<th>Name</th>
<th>Project</th>
<th>Supervisor</th>
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<tbody>
<tr>
<td>Olivia Highland</td>
<td>Synthesis of LDV peptide mimetics for the inhibition of the α4β1 integrin</td>
<td>Professor Luca Gentilucci</td>
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**Chemistry with a Year in Industry**

**FIRST**

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<thead>
<tr>
<th>Name</th>
<th>Project</th>
<th>Supervisor</th>
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<tbody>
<tr>
<td>Pierre Boufflet</td>
<td>Investigation of the transition-metal catalyst-free homopolymerisation of thiazole derivatives, and the synthesis of novel donor-acceptor copolymers based on bridged thiazole units</td>
<td>Dr Martin Heeney</td>
</tr>
<tr>
<td>Christopher Alan Brown</td>
<td>Synthesis of enantioenriched α-chloroesters through chiral counter ion and N-heterocyclic carbene cooperative catalysis</td>
<td>Dr Matthew Fuchter</td>
</tr>
<tr>
<td>Maddison Leigh Coke</td>
<td>The direct growth of cadmium sulphide nanoparticles through the annealing of cadmium precursor in solid state red absorbing polymer films for the use as hybrid solar cells</td>
<td>Dr Saif Haque</td>
</tr>
<tr>
<td>Katharina Reeh</td>
<td>Development of small-molecules targeting the Gad445β-MKK7 interface for multiple myeloma therapy</td>
<td>Dr Caroline Low</td>
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<tr>
<td>Guto Glyn Rhys</td>
<td>An approach towards the total synthesis of pseudopterosin aglycone A</td>
<td>Professor Donald Craig</td>
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**UPPER SECOND**

<table>
<thead>
<tr>
<th>Name</th>
<th>Project</th>
<th>Supervisor</th>
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<tbody>
<tr>
<td>Aurelio Arias</td>
<td>Towards photodynamic chemotherapy</td>
<td>Dr Matthew Fuchter</td>
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<tr>
<td>Ruth Patchett</td>
<td>Synthesis and characterisation of metal-organic frameworks with silicon containing organic linkers</td>
<td>Dr Paul Lickiss</td>
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<tr>
<td>Riten Solanki</td>
<td>Synthesis and catalytic studies of imidazolium-2-dithiocarboxylate complexes of palladium(II)</td>
<td>Dr James Wilton-Ely</td>
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**Chemistry with Medicinal Chemistry**

**FIRST**

<table>
<thead>
<tr>
<th>Name</th>
<th>Project</th>
<th>Supervisor</th>
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<tbody>
<tr>
<td>James Clarke</td>
<td>Assessment of a novel organocatalytic asymmetric macrobromolactonisation procedure for the synthesis of anti-malarial compounds</td>
<td>Dr Chris Braddock</td>
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<tr>
<td>Thomas Waugh</td>
<td>NMT Inhibitors against Leishmania</td>
<td>Professor Robin Leatherbarrow</td>
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Chemistry with Molecular Physics

**FIRST**

Omofolarin Oladipupo
DNA toroids: electrostatics and torsional adaptation
Professor Alexei Kornyshev

Nathan Francois Sengsiri
Bismuth sulfide as the light harvesting component in nanostructured solar cells
Dr Saif Haque

Scot Wheeler
An investigation into bulk heterojunction solar cell stability and the effect of interlayers
Professor James Durrant

**UPPER SECOND**

Andrew Yuk Keung Leung
Ordered inverse micellar lyotropic phases in phospholipid/alkanol/cholesterol mixtures
Professor John Seddon

**LOWER SECOND**

Seongmin Eun
The effect of electrolyte additives on the energy levels of the dye in dye sensitised solar cell
Dr Piers Barnes
<table>
<thead>
<tr>
<th>Name</th>
<th>Title of research project</th>
<th>Supervisor/s</th>
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<tbody>
<tr>
<td><strong>Bioimaging Sciences</strong></td>
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<tr>
<td>Aidan Ashton-Griffiths</td>
<td>Carbon-11 dithiocarbamate gold nanoparticles for PET imaging</td>
<td>Dr James Wilton-Ely and Dr Phillip Miller</td>
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<td>Yuko Isayama</td>
<td>Lanthanide functionalised gold nanoparticles for bioimaging</td>
<td>Dr James Wilton-Ely and Professor Jimmy Bell</td>
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<tr>
<td>Clare Leeson</td>
<td>Investigating functional thalamo-cortical connectivity</td>
<td>Dr Robert Leech and Dr David Sharp</td>
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<td>Henry Lovett</td>
<td>MRI contrast agents and PET tracers for the imaging of apoptosis</td>
<td>Professor Ramon Vilar and Professor Eric Aboagye</td>
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<tr>
<td>Emma Grenville-Mathers</td>
<td>The synthesis of metal-organic framework based contrast agents for magnetic resonance imaging enhancement</td>
<td>Dr Rob Davies and Professor Nick Long</td>
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<tr>
<td>Jonathan Nelson</td>
<td>Investigating compositions of lipid shell microbubbles for medical ultrasound imaging and therapy</td>
<td>Professor John Seddon and Dr Charles Sennoga</td>
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<tr>
<td>Luke Wainwright</td>
<td>Towards the synthesis of a dual-modal MRI-optical probe utilising the Cerenkov effect</td>
<td>Dr James Wilton-Ely and Professor Jimmy Bell</td>
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<td><strong>Chemical Biology of Crop Sustainability and Protection</strong></td>
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<td>Angela de Manzanos</td>
<td>Rubisco activase and rubisco structure function relationships – revealing regulatory mechanisms controlling photosynthetic efficiency</td>
<td>Dr Ian Gould, Dr Laura Barter, Dr James Murray and Dr Rudiger Woscholski</td>
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<tr>
<td>Saba Manzoor</td>
<td>A separation procedure of free Zn$^{2+}$ from complexed Zn-EDTA$^2-$ and determination of isotopic fractionation</td>
<td>Dr Dominik Weiss, Professor Ramon Vilar, Dr Thorsten Hamann and Professor Mark Sephton</td>
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<tr>
<td>Barany Sothirajah</td>
<td>Evaluating the role of pesticide use in bio-ethanol production from wheat in the UK</td>
<td>Dr Jeremy Woods and Dr Laura Barter</td>
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<td><strong>Chemical Biology of Health and Disease</strong></td>
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<tr>
<td>Ben Amor</td>
<td>A multiscale community detection method and random-walk network analysis uncovers allostERIC pathways in caspase-1</td>
<td>Dr Oscar Ces, Professor Sophia Yaliraki and Professor Mauricio Barahona</td>
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<tr>
<td>Natalie Andrews</td>
<td>Spatio-temporal mapping of enzyme activation in zebrafish using fluorescence lifetime optical projection tomography</td>
<td>Professor Maggie Daliman, Professor Paul French and Dr Andrew Thomas (AstraZeneca)</td>
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<tr>
<td>Pietro Aronica</td>
<td>Development of a new protocol for computational site-directed mutagenesis</td>
<td>Dr Ian Gould and Professor Robin Leatherbarrow</td>
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<tr>
<td>Michael Barclay</td>
<td>Single cell distributions: investigating the effect of Actinomycin D on p53 at the single cell level with the use of Microfluidic Antibody Capture (MAC) devices</td>
<td>Dr Oscar Ces and Professor David Klug</td>
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<tr>
<td>Rhianneon Beard</td>
<td>Oxytocin receptor imaging in the central nervous system: fluorine-18 tracer and delivery platform development</td>
<td>Dr Ed Tate and Professor Tony Gee</td>
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<tr>
<td>Ines Brizido</td>
<td>Capillary zone electrophoresis of PTEN coupled offline with an immunoassay</td>
<td>Professor David Klug, Dr Oscar Ces and Professor Keith Willison</td>
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<tr>
<td>Xiaoyu Chao</td>
<td>Cycloheptene-co complexes as potential tags for cu-free click reactions</td>
<td>Professor Alan Spivey and Professor Eric Aboagye</td>
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<tr>
<td>Marina Fedorova</td>
<td>Covalent immobilisation of the PTEN inhibitor V0-OHpic for determination of its biological targets</td>
<td>Professor Ramon Vilar, Dr David Mann, Dr Rudiger Woscholski and Dr Andrew Thomas (AstraZeneca)</td>
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<tr>
<td>Lays Gierakowski</td>
<td>Two-dimensional infrared spectroscopy as an analytical tool to study tyrosine nitration</td>
<td>Professor David Klug and Dr Oscar Ces</td>
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<tr>
<td>Edward Parsons</td>
<td>Towards a direct method for measuring interactions between proteins in opposing model membranes</td>
<td>Dr Jane Saffell, Professor John Seddon, Professor Paul Luckham and Professor Robin Leatherbarrow</td>
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<tr>
<td>Marcus Sims</td>
<td>Towards the development of fluorescent probes for imaging conformational changes in fibroblast growth factor receptors</td>
<td>Dr Ed Tate, Professor Paul French, Dr Chris Dunsby and Dr Andrew Thomas (AstraZeneca)</td>
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<tr>
<td>Ernest So</td>
<td>Chemical AMPylinomics: understanding critical host-pathogen interactions in bacterial infection</td>
<td>Dr Ed Tate and Professor Gadi Frankel</td>
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<tr>
<td>Peter Thomson</td>
<td>Synthesis of a new zinc-coordinating ligand and a method to assay zinc uptake by cells for investigating Akt Activation by Zinc</td>
<td>Professor Ramon Vilar, Dr Rudiger Woscholski and Professor David Klug</td>
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<tr>
<td>Ben Turner</td>
<td>Study of biologically relevant molecular complexes using two-dimensional infrared spectroscopy</td>
<td>Professor David Klug and Professor Steve Matthews</td>
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<tr>
<td>Jennifer Ward</td>
<td>Activity-based protein profiling of E3 ubiquitin ligases in the DNA damage response</td>
<td>Professor Eric Lam, Dr Ed Tate, Matt Fuchter and Dr Andrew Thomas (AstraZeneca)</td>
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<tr>
<td>Juliet Wilcox</td>
<td>Design, synthesis and activity profiling of modified 3-and 5-hydroxypicolinic acid vanadyl complexes against PTEN as models for targeted probes</td>
<td>Professor Robin Leatherbarrow, Professor Ramon Vilar and Dr Rudiger Woscholski</td>
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<tr>
<td>Daniel Wilkinson</td>
<td>Electrochemical aptamer biosensors: screen printed electrodes as a cost effective disposable electrode system</td>
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<tr>
<td>Doug Wylie</td>
<td>Novel micro-delivery systems: through live single cell membranes and beyond</td>
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**Drug Discovery and Development**

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<tr>
<th>Name</th>
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<tbody>
<tr>
<td>Amal Althubiti</td>
<td>Structural and binding study of ochratoxin- AS1411 fusion aptamers to nucleolin to be used as a drug delivery into cancercells</td>
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<tr>
<td>David Cooney</td>
<td>Identification of inhibitors of p90 ribosomal S6 kinase</td>
</tr>
<tr>
<td>Nino Gaphrindasvili</td>
<td>Hedgehog acyltransferase as a drug target in cancer</td>
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<tr>
<td>Louis Perdios</td>
<td>Mapping and sequence identification of multiple alpha-catatin binding sites within the TBC/RabGAP Armus</td>
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<tr>
<td>Daniel Perks</td>
<td>Synthesis and biological activity of potential gemcitabine pro-drugs formed by bile acid conjugation</td>
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<tr>
<td>Yunyun Sun</td>
<td>Towards stapled peptides for inhibiting the malarial invasion motor complex</td>
</tr>
<tr>
<td>Tiffany Teng</td>
<td>The effect of specific histone deacetylase inhibitors in attenuating pulmonary arterial hypertension</td>
</tr>
<tr>
<td>Wenting Wu</td>
<td>Validation of sphingosine kinase-1 Inhibitors as potential new antifungal treatment</td>
</tr>
<tr>
<td>Emmanouil Zacharioudakis</td>
<td>The design and synthesis of novel SIRT2 inhibitors</td>
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**Green Chemistry**

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<tr>
<th>Name</th>
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<tr>
<td>Okpara Bull</td>
<td>Combating climate change: new technologies for carbon dioxide capture</td>
</tr>
<tr>
<td>Junzi Li</td>
<td>Lignocellulosic biomass fractionation with ionic liquids and liquid acid mixtures</td>
</tr>
<tr>
<td>Peilin Li</td>
<td>Ionic liquids for converting lignin to biopolymers</td>
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<tr>
<td>Thanit Montrikittiphant</td>
<td>Degradable and renewable polymers and composites</td>
</tr>
<tr>
<td>Rebecca Sherwood</td>
<td>Catalytic magnetic nanoparticles</td>
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**Nanomaterials**

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<tr>
<th>Name</th>
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<tbody>
<tr>
<td>Karan Agarwal</td>
<td>Separation CNT based on their metallic and semiconducting properties</td>
</tr>
<tr>
<td>Harini Hewa Dewage</td>
<td>Synthesis and characterization of metal-organic frameworks: nano-sized fuel tanks</td>
</tr>
<tr>
<td>Yajie Gao</td>
<td>The role of nanocrystalline glass-ceramic dental materials</td>
</tr>
<tr>
<td>Chauan–Wen Kuo</td>
<td>Ion transport in ionic liquids</td>
</tr>
<tr>
<td>Iris Kramberger</td>
<td>Single-molecule heaters for biomedical intervention</td>
</tr>
<tr>
<td>Charles-Henri Lambert</td>
<td>Theory of nanomagnetism</td>
</tr>
<tr>
<td>Ashley Senior</td>
<td>Nanoseparations using metal organic frameworks</td>
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**Plastic Electronics**

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<tr>
<th>Name</th>
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<tr>
<td>Abby Casey</td>
<td>Light absorbing donor materials for OPV</td>
</tr>
<tr>
<td>Joshua Green</td>
<td>Non-invasive sensors for the detection of diabetes via breath samples</td>
</tr>
<tr>
<td>Sarah Holliday</td>
<td>Low LUMO polymeric electron acceptors</td>
</tr>
<tr>
<td>Thomas Phillips</td>
<td>Development of new interlayer materials and processes</td>
</tr>
<tr>
<td>Karananantharajah Prashanthan</td>
<td>Characterization of polymer – metal oxide nanocomposite films for hybrid solar cells</td>
</tr>
<tr>
<td>Name</td>
<td>Title of Thesis</td>
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<tr>
<td>Mohd Azri Ab Rani</td>
<td>Synthesis, characterization and physical-chemical properties of room temperature ionic liquids with a variety of cations, paired with bis(trifluoromethylsulfonyl)imide anion</td>
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<tr>
<td>Nurul Huda Abd Karim</td>
<td>Studies towards elucidating the binding modes between metal-salphen complexes and G-quadruplex DNA</td>
</tr>
<tr>
<td>Mohd Firdaus Abdul Wahab</td>
<td>Mechanistic behaviour and molecular interactions of heat shock protein 47 (HSP47)</td>
</tr>
<tr>
<td>Kai Helmut Abersfelder</td>
<td>Stable partially substituted silicon clusters from functional disilenes and homo- and heterocyclic silanes</td>
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<tr>
<td>Jannine Arbour</td>
<td>Metal-mediated intramolecular hydroamination and hydro(acyl)alkoxylation reactions</td>
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<tr>
<td>Alessia Arduin</td>
<td>Interactions of phosphoinositide specific phospholipase C with a lipid layer for structural and functional studies</td>
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<tr>
<td>Beeta Balali-Mood</td>
<td>Uniquely branched and structurally versatile lanthanide-based contrast agents for MRI</td>
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<tr>
<td>Shah Mohammad Abdul Baten</td>
<td>Optical second harmonic generation studies of electrochemical interfaces</td>
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<tr>
<td>Matthias Gerard Jacky Baud</td>
<td>Towards novel small molecule epigenetic inhibitors</td>
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