Imperial College London is a world leading University. In 2008 the Times Higher Education Supplement placed us 3rd in Europe and 5th in their World University Rankings. As the central science Chemistry has been a major contributor to this success. We were also ranked 3rd in Europe and 1st in the UK for ‘impact’ (average citations per paper for the decade to February 2009) in Chemistry by Thomson Reuters Essential Science Indicators database.

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 2009 they won a total of seven internationally recognised scientific awards. This is made possible by the superb researchers and students in the Department, who do most of the hard work. From professors to students, we are proud to be a diverse community who come from all across the globe.

We are particularly proud of the award of a Royal Society Athena Swan Silver Award for good practice in supporting academic women. This award recognised the good practices already in place for supporting not only women, but all of our staff and students, and the plans for future developments. These stem from our belief that world leading science is done by world leading scientists and that it is only by helping each other to reach our full potential as scientists that the Department can achieve its aim of being the first choice destination to study and research Chemistry.

This review gives a snapshot of some of our research activities in 2009. 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

Tom Welton
Head of the Department of Chemistry
Imperial College London
2009 was another successful year for the Department of Chemistry. In this review you will be able to see the great breadth and depth of our research activities. In addition to this I would like to tell you of some of the highlights of the year.

Honours and Awards
The Department received two awards from the American Chemical Society's History Division at a half-day symposium in honour of the seminal works of Professors Wilkinson and Barton.

**Professor Andrew de Mello**, Head of the Nanomaterials and Devices Section, was invited to give the prestigious Royal Society Clifford Paterson Lecture.

**Dr David Scheschkewitz** was awarded the Carl Duisberg Memorial Prize for his contributions towards the application of Si=Si moieties as functional units in conjugated materials. The Carl Duisberg Memorial Prize has been awarded since 1935 to young investigators of all chemical disciplines to honour the memory of the industrial chemist Carl Duisberg.

The Department of Chemistry won five RSC awards this year, more than any other chemistry department in the UK, these were award for:

- **Dr Fernando Bresme** RSC/SCI McBain Medal
- **Professor James Durrant** RSC Environment Prize
- **Professor Iain McCulloch** RSC Creativity in Industry Prize
- **Professor Andrew de Mello** RSC Corday-Morgan Prize
- **Professor Donna Blackmond** RSC Physical Organic Chemistry Award

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**Dr Marina Kuimova**, EPSRC Research Fellow, was awarded the Roscoe medal for the best Chemistry poster and also the Westminster medal for the best poster at a SET for Britain Early Career Researchers Event held at the Houses of Parliament in March 2009.

**Dr Paul Wilde** received a Rector's Excellence in Teaching Award (2008-09). These annual awards are granted to staff judged to have been most outstanding in the quality, organisation and presentation of their teaching.

The Department was awarded a Royal Society Athena Swan Silver Award for good practice in supporting academic women. This award recognises the good practices already in place for supporting women at all stages, including undergraduate, post graduate, post doctoral, and early career academic through to professorial level. The Athena judges highlighted that the Department has “demonstrated that there was real change going on” and that the plan of activities developed to support, enhance and reward women at all stages within the department “was clear and comprehensive”, and they congratulated “the Department of Chemistry at Imperial College London on an impressive submission...”

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**Research Fellowships**

**Dr Ramon Vilar**, Reader in Inorganic Chemistry was awarded a five-year EPSRC Leadership Fellowship.

**Dr John de Mello**, Reader in Nanomaterials was awarded a three-year Royal Society Industrial Fellowship.

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**External appointment**

Former Head of Department and Emeritus Professor David Phillips OBE was confirmed as President-Elect of the Royal Society of Chemistry and will take up his position fully in July 2010.

**New Members of Academic Staff**

2009 saw a bumper crop of new academics coming to the Department. This was partly boosted by the introduction of the Imperial Junior Research Fellows scheme. These are awarded to young scientists of outstanding potential.

**Dr Martin Heeney**, Senior Lecturer

Martin is a graduate of the University of East Anglia, and received his PhD from the same institution in 1999 under the supervision of Professor Michael Cook. Following a postdoctoral position with a start-up company in the area of photodynamic therapy, he joined Merck Chemicals in 2000, becoming project leader for the organic electronics team. After seven years in industry, he decided to return to academia and joined the Materials Department at Queen Mary University of London in October 2007, before moving to his current position in May 2009. His current research interests include the synthesis and properties of conjugated oligomers and polymers for a variety of optoelectronic and sensing applications.

**Dr James Wilton-Ely**, Lecturer

James joined Imperial in 2009 as a Lecturer in Inorganic Chemistry after independent research positions as Fitzjames Fellow at the University of Oxford (Merton College) and Ramsay Fellow at UCL. He is no stranger to the Department as he received both BSc and PhD degrees (the latter with Professor A F Hill) at Imperial before undertaking postdoctoral research in Munich (Professor H Schmidbaur) and University of St Andrews (Professor D J Cole-Hamilton). This background provided...
the extensive experience in coordination and organometallic chemistry, which underpins much of his research activity. As well as more traditional synthetic transition metal chemistry, current interests include the immobilisation of transition metal units on the surface of gold nanoparticles for applications in catalysis and sensing of anions. This research into nanoscale materials extends also to functionalised thiols for the preparation of Self Assembly Monolayers (with Dr M Buck, University of St Andrews).

Dr Silvia Díez-González, Junior Research Fellow
Silvia completed her PhD at the Université Paris XI (France), before joining the research group of Professor Steven P Nolan at the University of New Orleans (USA) as a post-doctoral fellow. Due to the harsh weather conditions in New Orleans, and after a brief stay at the University of Ottawa (Canada), she followed Professor Nolan to the Institute of Chemical Research of Catalonia (ICIQ) in Spain, where she was offered a position as Group Coordinator. During this period she was also awarded a Torres Quevedo Research Fellow. Having established metal-mediated reactions as her main research interest, in 2009 she explored this field from a computational perspective in the group of Professor Feliu Maseras at the ICIQ. In October 2009, and against all forecasts, Silvia left sunny Tarragona to join the Department of Chemistry as part of the first round of Imperial Junior Research Fellows. At present, her research themes rely on the use of pre-formed catalysts as tools for developing greener processes and bringing some light on the so-called blackbox of catalysis.

Dr Nick Evans, Junior Research Fellow
Nick completed a BSc in chemistry at Massey University (1998–00) before working for one year in industrial carbohydrate chemistry in New Zealand. He was awarded a Commonwealth Scholarship to pursue doctoral studies at the University of Cambridge (2001–04) under the supervision of Professor Andrew Holmes in the field of phosphorescent conjugated polymers for organic light-emitting diodes (OLEDs). Postdoctoral positions followed at the Ecole Polytechnique Fédérale de Lausanne (2005–07) with Professor Michael Grätzel in the fields of dye-sensitised solar cells, lithium-ion batteries and OLEDs and at Imperial (2007–09) with Dr Charlotte Williams in the field of conjugated polymers. He was awarded an Imperial Junior Research Fellowship in 2009.

Dr James Bull, Ramsay Memorial Fellow
James completed both MSci and PhD degrees at the University of Cambridge (Professor Steven V Ley CBE FRS FMedSci), separated by a year spent as a Research Scientist at GlaxoSmithKline working in medicinal chemistry. In 2007 he took up a postdoctoral position at the Université de Montréal in Canada (Professor André B Charette) where he was involved on a range of synthesis projects, particularly involving organometallic intermediates. After two Montreal summers (and winters!) he decided to return to the UK to begin independent research. In October 2009 he joined Imperial College London as a Ramsay Memorial Research Fellow (2009–11), working in the laboratories of Professor Alan Armstrong. Dr Bull has broad research interests in the area of synthetic organic chemistry, with a focus on the construction of important heterocyclic structures.

Dr Ruth Martínez Casado, Newton Fellow
Ruth obtained her BSc in Physics in 2003 (Universidad Autonoma de Madrid, Spain). After that she got two MSc, one in Biophysics and another in Condensed Matter Theory, before starting her PhD on the study of He-atom scattering from surfaces. This was a joint project between the Bochum University (Germany) and the Spanish Research Council (Spain).

Dr Martínez-Casado was awarded her PhD in 2008 (Universidad Autonoma de Madrid, under the supervision of Professor Salvador Miret-Artes and Dr Angel S Sanz Ortíz). In the same year she was awarded a Newton International Fellowship by the Royal Society and joined Professor Nicholas Harrison’s group in the Department of Chemistry at Imperial College London. The main aim of her Newton project consists of shedding some light on the first-principle description of He-surface interaction potentials, which is at present a central problem in the theoretical interpretation of He-atom experiments. This work is being carried in direct collaboration with experimental groups in Germany and the UK, and is intended to make a major contribution in extending the use of He-atom scattering to a very wide scientific community.

Dr Dong-Ku Kang, Newton Fellow
Dong-Ku completed his PhD in Biochemistry and Molecular Biology in 2006 (Chungbuk National University, Professor Soo-Ik Chang). He then took up a Research Associate position there for about two years focussing his research on proteomics using protein micro/nano-array for inhibitor screening of protein-protein interaction.

In November 2009 he was awarded a Newton International Fellowship by the Royal Society and took up his position in the Nanostructured Materials and Devices Group at the Department of Chemistry, Imperial College London. His research is currently focused on biological application using microfluidic devices.

2009 Alumni Day
In September 2009, Imperial held its annual alumni day. Head of Department Professor Tom Welton gave a tour of the Department to a number of Chemistry alumni and this was followed by a reception. The Department of Chemistry looks forward to welcoming more alumni in September 2010.

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
- Using solvent effects and environmentally friendly solvents
- Fast and targeted synthesis for medical imaging

Current activities in materials include:

- Biodegradable materials
- Biosustainable polymers
- Electroluminescent metal-containing materials
- Organometallic polymers
- Polyoelfins
- 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 Oscar Ces, Dr Ian Gould, Professor David Klug, Dr Rob Law, Professor Robin J Leatherbarrow (Head of Section), Dr Joachim Steinke, Dr Ed Tate, Professor Richard Templer, Dr Ramon Vilar and Dr 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).
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 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 innovation. Research also includes the development of sustainable synthetic chemistry including catalytic enantioselective and atom economic reactions and the use of non-traditional solvents including ionic liquids. The synthesis and computational studies of dendrimers, speciality polymers, including conjugated polyaromatics, heterocyclic block copolymers, ring opening metathesis polymers and modified lactic acid, 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 monomeric and oligomeric low value silicon species such as silenes and disilenes, as well as derived transition metal complexes, novel bridged main group element cations, mesoporous solids and silsesquioxanes for hydrogen storage, bimetallic cuprate reagents and alkene metathesis reactions. High performance bimetal chalcogenolates and heterobimetallic early transition amides and phosphinimides are being synthesised as single source chemical vapour deposition (CVD) precursors. 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
- Silenes and Disilenes, oligomers and polymers
- Discovery of advanced precursors for CVD
- Synthesis of multimetallic assemblies
- Optoelectronic properties of low-valent main-group compounds
- Synthesis of metal-organic framework materials for hydrogen storage
- Removal of siloxanes from biogas
- 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, Dr David Scheschkewitz and Professor Alan Spivey
alkene aziridination procedure, proceeding via aminemine.

Aziridines are highly useful synthetic building blocks and provide access to vinyl glycine derivatives, and are exploring amination/sigmatropic rearrangement of allylic sulfides which recently developed a novel, efficient and highly stereoselective asymmetric synthesis involving nitrogen transfer. They have following on from this work in the development of new catalysts of air or water, and they avoid the use of potentially toxic organocatalysis. Organocatalytic reactions have the advantage of small organic molecules as catalysts, an area known as armstrong and his group span a range of different areas from single-molecule conductance studies in molecular electronics to ion and biopolymer transport in small solid-state nanopores. In the former, scanning tunnelling microscopy in electrochemical environments (ECSTM) is one of the key tools; by means of multi-dimensional tunnelling spectroscopy as a unique feature of ECSTM, it is possible to probe electron transport mechanisms and dynamics on the single-molecule level and at an unprecedented level of detail. We have studied a wide range of target systems, including small inorganic transition metal complexes, redox-modified DNA, and gold nanoparticles, in aqueous solvents and ionic liquids. Each of these holds interesting new features, such as single-molecule diode and transistor characteristics (‘electrochemical gating’), elements of coherent electron transfer, dielectric saturation and sequential charging. A second area of interest focuses on ion and biopolymer transport in electrode/nanopore architectures for applications in biosensing, integrating electrochemical concepts with solid-state nanopores. Examples include the fabrication of ultra-small metallic nanopores, the integration of local electrochemical gates, and fast switching schemes.

2009 Publications

Zuo P, Albrecht T, Barker PD, Murgida DH and Hildebrandt P
Interfacial redox processes of cytochrome b562

Professor Alan Armstrong
(Synthesis)

As part of the synthesis section, Professor Alan Armstrong’s work focuses on the development of new synthetic methodology and its application to target synthesis, including compounds to probe biological pathways. Underpinning this work are studies on the mechanisms of organic reactions by kinetics and computational studies. In asymmetric synthesis, 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 this work in the development of new catalysts for alkene epoxidation, the group are currently focusing on asymmetric synthesis involving nitrogen transfer. They have recently developed a novel, efficient and highly stereoselective amination/sigmatropic rearrangement of allylic sulfides which provides access to vinyl glycline derivatives, and are exploring further applications of this concept.

Aziridines are highly useful synthetic building blocks and the group have recently developed a novel aminemated alkene aziridination procedure, proceeding via aminemine intermediates. Optimisation of catalyst turnover and asymmetric induction are underway. The group are involved in protein-ligand engineering studies for the elucidation of the roles of specific kinases and phosphatases, proteins which have key roles in the anti-cancer area. These studies are inspired by natural product leads and require efficient synthetic approaches to natural products and their analogues.

2009 Publications

Dhill Ws, Bewick GA, White NE, Gardiner JV, Thompson EL, Batavelic A, Murphy KG, Roy D, Patel NA, Scott JN, Armstrong A, Ghatel MA and Bloom SR
The thyroid hormone derivative 3-iodothyronamine increases food intake in rodents
Diabetes Obes. Metab. 2009, 11, 251

Armstrong A and Emmerson DPG
Enantioselective Synthesis of Allenamides via Sulfinide
[2,3]-Sigmatropic Rearrangement
Org. Lett. 2009, 11, 1547

Armstrong A, Ashraff CA, Chung H and Murtagh L
Oxidative Rearrangement of 2-Alkylx-3,4-dihydro-2H-pyran: Stereocontrolled Synthesis of 4,5-cis-Disubstituted Tetraydrafuranylenes including Whisky and Cognac Lactones and Croobarbic Acid
Tetrahedron, 2009, 65, 4490

Armstrong A and Pyrkotis C
Synthetic studies on Amphidinolides C and F: Synthesis of the C18-C29 Segment of Amphidinolide F

Zotova N, Broadbelt LJ, Armstrong A and Blackmond DG
Kinetic and Mechanistic Studies of Proline-Mediated Direct Intermolecular Aldol Reactions

Armstrong A, Bhonoah Y and White AJP
Constrained β-Proline Analogues in Organocatalytic Aldol Reactions: The Influence of Acid Geometry
J. Org. Chem. 2009, 74, 5041

Zotova N, Moran A, Armstrong A and Blackmond DG
A Coherent Mechanistic Rationale for Additive Effects and Autoinductive Behavior in Proline-Mediated Reactions

Professor Anthony G M Barrett (Synthesis)

Total synthesis of natural products; catalysed organic transformations; synthesis and biological evaluation of anti-cancer compounds; imaging agents for the early-stage detection of disease.

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 antibiotic quinone and aromatic natural products including clavilactone B, citrafungin A, Sch 47554, lactonamycin and 15G2568. Methodology that has been developed includes highly enantio- and diastereo-selective routes to vinylcitrilate derivatives, the iterative use of the Michael addition reaction to prepare polycyclic aromatic systems and the application of double benzynes for the two-directional synthesis of anthraquinones. Finally, in unpublished research the group...
has shown that macrocyclic resorcylic natural products are readily available from simple dioxinone precursors using mild late-stage aromatisation.

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 nitrations 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 apicidin analogues. Finally, in collaboration with Dr Mike Hill, he has applied alkaline earth catalysts for hydroaminations, hydrophosphinations and other important reactions.

The Barrett group in collaboration with B.M. Hoffman at Northwestern University have synthesised new classes of porphyrazines and seco-porphyrinazines. 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. Porphyrin inorganic complexes 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 multi-metallic 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.

### 2009 Publications

**Zong H, Sun P, Mirkin CA Barrett AGM and Hoffman BM**  
Varying the Electrochemical Potential and Thickness of Porphyrazine SAMs by Molecular Design  

A ‘push-pull’ tropylium-fused aminoporphyrine  
Tetrahedron, 2009, 65, 9690-9693

**Crimmin MR, Mark R, Barrett AGM, Hill MS, MacDougall DJ, Mahon MF and Procopiou PA**  
beta-Diketiminate C-H activation with heavier group 2 alkyls  
Dalton Transactions 2009, 9715-9717

**Navarro I, Poverlein C, Schlingmann G and Barrett AGM**  

**Calo F, Richardson J and Barrett AGM**  
Total Synthesis of Aigialomycin D using a One-Pot Ketene Generation-Trapping-Aromatization Sequence  
Organic Letters, 2009, 11, 4910-4913

**Barrett AGM, Brinkmann C, Crimmin MR, Hill MS, Hunt P and Procopiou PA**  
Heavier Group 2 Metals and Intermolecular Hydroamination: A Computational and Synthetic Assessment  
Journal of the American Chemical Society, 2009, 131, 12906

**Goslinski T, Zhong C, Fuchter MJ, White AJP, Barrett AGM and Hoffman BM**  
Serendipitous synthesis of trimetallic porphyrazine triads  

The Development of a Selective Cyclin-Dependent Kinase Inhibitor That Shows Antitumor Activity  
Cancer Research, 2009, 69, 6208-6215

**Crimmin MR, Arrowsmith M, Barrett AGM, Casely II, Hill MS and Procopiou PA**  
Total synthesis and determination of the absolute stereochemistry of the squalene synthase inhibitors CJ-13,981 and CJ-13,982  

**Barrett AGM, Casely II, Crimmin MR, Hill MS, Lachs JR, Mahon MF and Procopiou PA**  
b-Diketiminate Calcium and Magnesium Amides; Model Complexes for Hydroamination Catalysis  
Inorganic Chemistry, 2009, 48, 4445-4453

**Barrett AGM, Crimmin MR, Hill MS, Hitchcock PB, Lomas SL, Procopiou PA and Suntharalingam K**  
Catalytic 2,3,4-hexatriene formation by terminal alkyne coupling at calcium  
Chemical Communications, 2009, 2299-2301

**Calo F, Richardson J, White AJP and Barrett AGM**  
Enantioselective formal total synthesis of (-)-trachyspic acid  

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**Dr Laura Barter (CB)**

Dr Laura Barter’s broad interests involve determining quantitative structure function relationships in biological systems by employing optical spectroscopic, biochemical and proteomic techniques allied with modelling and calculation. Her particular focus is on Photosynthetic inefficiency. Barter is a Royal Society Research fellow, and has recently had her fellowship renewed.

Understanding the inefficiencies of Photosynthesis: Climate change means that there will be an increasing reliance on carbon-neutral liquid fuels and bioproducts derived from plants. In order to meet this demand there is a pressing need to increase plant yield, and resilience. Higher plant photosynthetic efficiency is only ~1% whereas the theoretical maximum is thought to be ~6-8% giving the potential for great improvements. However, it is not clear where in the photosynthetic process that the additional losses are occurring. Dr Barter’s research group employs a combination of spectroscopic methods, proteomic tools and computational modelling to reveal pathways, mechanisms and rate limiting steps that control the light dependent and dark Photosynthetic reactions.

Dark Photosynthetic reactions: Inside plant cells, a network of enzymes creates organic carbon from the CO2 in the air and these reactions are strikingly inefficient. Typical enzymes can process ~1000 molecules per sec, but one of the enzymes,
Rubisco, involved in the network, fixes only about 3 CO2 molecules per sec. This research program aims to improve understanding of the inefficiency of photosynthesis, focusing on the dark cycle enzymes and in particular Rubisco. An understanding of Rubisco's inefficiency could clearly have significant impact, as it may provide a route to achieving profound improvements in photosynthetic efficiencies, through manipulating Rubisco in the chloroplast of higher plants.

This requires a range of quantitative approaches if the delivery of selected or engineered traits is to be a viable proposition. Professor David Klug, Professor Martin Parry ( Rothamsted Research Institute) and Dr Laura Barter have students working on quantitative proteomics, metabolomics, transcriptomics all allied with modelling and calculation to probe the Rubisco interactome and to investigate the regulatory networks controlling photosynthetic efficiency. The aim being to determine how these interactions control the up and down regulation of the enzyme. Initial studies are currently being made using conventional proteomic methods. The ultimate aim of this project is to investigate the Rubisco interactome using 2DIR spectroscopy as a proteomic tool, as this should offer both high sensitivity and throughput.

Photosynthetic water splitting: The chloroplast houses a membrane which contains a chain of complexes involved with the intake of light energy and the transfer of charge across the membrane. This separation of charge is a method of storing energy and can be thought of as being like a battery, and therefore these complexes are the power-house of the organism. It is striking that the plant is able to store enough energy, by creating stable intermediate states, to drive the energy demanding reactions that split water and release oxygen as a byproduct. These reactions occur over timescales that cover more than fifteen orders of magnitude. A range of spectroscopic methods in combination with modeling allow us to probe the quantitative structure function relationship.

Single molecule spectroscopy has also been employed to probe heterogeneity and dynamics associated with steps hidden by rate limiting processes in an ensemble experiment properties of Photosynthetic complexes that are inaccessible in any other way. In particular the work has focused on the heterogeneity of the process and the dynamics associated with steps hidden by rate limiting processes in an ensemble experiment.

Two-Dimensional Infrared Spectroscopy: In collaboration with Professor David Klug, research includes use of an optical analogue of 2D NMR to measure vibration-vibration coupling which is being developed so that it can be employed as a novel sensitive proteomic tool. This will be employed to probe the dark cycle enzyme interactome.

Biofuel analysis: In collaboration with Dr Preben Krabben (Green Biologics) and Professor Jeremy Nicholson (Imperial), Barter is investigating the use of metabolomic analysis as a diagnostic tool in the biofuel industry. Particular use is likely to be during process development and also as a commercial control diagnostic tool during the fermentation process. Work is currently focusing on the analysis of samples from the production of butanol from biomass.

Capture and Detection of CO2 by Carbonic Anhydrase Mimics: Carbon dioxide is a natural by-product of catabolic metabolism. Carbonic anhydrases provide a regulatory control over the equilibrium between CO2 and its hydrated form. This project is in collaboration with Professor Nicholas Long and Dr Woscholski (Div of Cell and Molec. Biol). Using established chemistry from the Long group, a new metal-based CO2 binding compound will be the initial target. The novel compounds will be tested with respect their specificity and affinity, by the Barter group, who will employ Rubisco based assays to test the inhibitory potency of the CO2 binding compounds.

EPSRC Cross-Disciplinary Feasibility Account entitled ‘Elements of a Vesicle Machine’: This is a collaborative project with Professor Richard Templer, Dr Oscar Ces, Dr Rob Law, Professor John Seddon, (Imperial College London); Dr Mark Wallace, (Oxford); Professor George Attard, (Southampton); Professor Paula Booth, (Bristol). It is investigating how self-assembling amphiphilic structures and various sub-cellular components can be coupled together to make hybrid, self-sustaining microscale machinery capable of acting as power sources. The behaviour of vesicles implanted with either chloroplast and/or mitochondrion power sources will be investigated.

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, we showed that introduction of a second charged residue (deprotonation of Glu81) into the retinal-binding pocket lead to remarkably small differences in key properties, particularly the S0→S1 and S0→S2 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, and the Gaussian code released in 2009 features contributions from the group.

Earlier calculations by the group showed how the shape and accessibility of crossings of potential energy surfaces determine 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 hydrocarbons found in the interstellar medium, such as perylene radical cation. Algorithm and code developments carried out in the group remain central to these investigations, suggesting ways of designing molecules to be photostable.

State crossings are also crucial for the successful operation of photochromic molecules: a series of articles co-authored since 2002 have provided a systematic way of understanding and predicting 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.
2009 Publications

Araujo M, Lasorne B, Magalhaes AL, Worth GA, Bearpark MJ and Robb MA
The molecular dissociation of formaldehyde at medium photoexcitation energies: A quantum chemistry and direct quantum dynamics study
Journal of Chemical Physics, 131, Article Number: 144301 (2009)

Larkin SM, Vreven T, Bearpark MJ and Morokuma K
The application of the ONIOM hybrid method to the cycloaddition reactions of bromo-substituted 2(H)-pyran-2-ones(1)

Blancfart L, Lasorne B, Bearpark MJ, Worth GA and Robb MA
Second-Order Analysis of Conical Intersections: Applications to Photochemistry and Photophysics of Organic Molecules

Frisch et al, Gaussian 09, Revision A.02

Dr Chris Braddock (Synthesis)

The Braddock Group is engaged in stereoselective synthesis, organocatalysis, aspects of transition metal catalysis, and natural product synthesis. In particular, we are working towards a general organocatalytic asymmetric reaction of alkenes for the preparation of diverse 1,2-difunctionalised building blocks, and exploiting biomimetic electrophilic bromination for a diversity orientated approach to halogenated natural products such as the obtusallenes, and medium ring ethers from Laurencia species as both supported by the EPSRC.

The calendar year of 2009 has seen a publication in Chemical Communications detailing the first generation and trapping of an enantiopure bromonium ion. This research output by the Braddock group establishes that such species can be generated and trapped without compromising their stereochmical purity and is a new milestone in the history of the bromonium ion. This work provides a solid platform for further development of a catalytic asymmetric bromination reaction of alkenes.

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 biomimetic transannular rearrangement in model obtusallene systems as driven by formation of a bromonium ion. This is consistent with our published hypothesis on the biogenesis of these metabolites and was published as a Featured Article in this journal. It also allowed the reassignment of structures of obtusallenes V-VII on the basis of a chlorine-induced isotope effect. This research now allows us to target the total synthesis of the entire obtusallene family with confidence in this approach.

In collaboration with Dr Jonathon Burton at Oxford University, our two research groups have clarified the stereochmical course of nucleophilic substitution of arylsulfonate-based nucleophile assisting leaving groups. Previous work from other research groups suggested that a SN1 mechanism could be operating with such leaving groups. A comprehensive investigation of this provocative suggestion showed instead that the ‘normal’ routes of SN2 or SN1 substitution operate depending on the reaction conditions employed. Any observed retention of configuration is likely due to neighboring group participation or diastereoselective attack on a carbothion (or ion pair) rather than an SN2 mechanism. This research was also published as a full article in the Journal of Organic Chemistry.

Dr Fernando Bresme (CP)

Dr Fernando Bresme’s research is concerned with the investigation of soft interfaces. Soft interfaces appear in many problems of interest in chemistry, physics and biology: colloids, biopolymers, membranes, nanomaterials. These are the building blocks of many devices used in current nanotechnology applications. Soft interfaces are characterized by 1) the complexity of their constituents, often involving macromolecular entities, and 2) the ability of these constituents to self-organize into complex structures. One essential element of soft matter is the strength of the interactions between different components, which are of the order of the thermal energy. Consequently thermal fluctuations play a very important role in determining the self-assembly process into structures that often exhibit striking properties not found in other condensed phases (e.g., liquids and solids). Many soft materials involve interfaces that determine to a great extent the physical and chemical behaviour of the overall system.

Dr Bresme’s group develops and applies computational methods and theoretical approaches to understand and interpret the behaviour of soft interfaces. Their research focuses on three main topics: 1) interactions between nanoparticles and biomolecules at liquid-liquid and liquid-vapour interfaces, and how these interactions can be exploited to design interfacial molecular devices that can respond to external perturbations (e.g. external magnetic fields). 2) Structure and phase behaviour of soft materials (polyelectrolytes and membranes), with particular emphasis on the role of the solvent in determining their properties and 3) Non equilibrium phenomena at nanoscale interfaces, in particular, the investigation of energy transfer processes across interfaces of relevance in high performance materials (e.g. nanofluids).
2009 Publications

Lervik A, Bresme F and Kjelstrup S
Heat transfer in soft nanoscale interfaces: the influence of interface curvature

Bresme F, Lehle H and Oettel M
Solvent-mediated interactions between nanoparticles at fluid interfaces
Journal of Chemical Physics, Volume: 130, 214711 (2009)

Alejandre J, Chapela GA, Bresme F and Hansen
The short range anion-H interaction is the driving force for crystal formation of ions in water


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

2009 Publications

Whiteoak C, Britovsek GJP, Gibson VC and White AJP
Electronic Effects in Oxo Transfer Reactions Catalysed by Salan Molybdenum(VI) cis-dioxo Complexes
Dalton Trans., 2009, 2337-2344

Dalton Trans., 2009, 5319-5334

Taylor RA, Law DJ, Sunley GI, White AJP and Britovsek GJP
Towards Photocatalytic Alkane Oxidation: The Insertion of Dioxgen into a Platinum(II)-Methyl Bond

Dr James Bull (Synthesis)

Dr James Bull’s research focuses on the development of new synthetic methodology to access complex organic structures.

The development of new and improved methods of chemical synthesis is essential to enable efficient access to small-molecules for an increasing range of applications. Dr Bull is interested in the development of reactions that generate complexity in low molecular weight systems to provide important structural units with high yields and stereocntrol. Specifically, approaches are targeted to access core functional units that i) contain biologically important motifs or ii) function as synthetic intermediates.

WITH THESE THEMES, CURRENT RESEARCH IS DIRECTED ALONG TWO LINES:

• Synthesis of heterocyclic rings; 3- and 4-membered rings and aromatic heterocycles relevant to medicinal chemistry and chemical biology applications. For example, a synthesis of activated aziridine species for the stereoselective construction of diverse derivatives is currently being developed.

• Synthesis of halogenated compounds as versatile intermediates in organic synthesis.

Central to the research strategy is the development of the synthetic applications of organometallic reagents, particularly alpha-halo metal species, organoboron reagents and transition metal-catalysed cross-coupling methodology.

Dr Bull joined the department in October 2009 as a Ramsay Memorial Research Fellow based in the laboratories of Professor Alan Armstrong. His previous work developed novel reaction methodologies and their application to the synthesis of complex structures and natural products. He developed the first intramolecular Simmons-Smith (IMSS) cyclopropanation reaction, as well as a synthesis of geminal-diiodoalkanes and a novel synthetic approach to styril halides (with Professor André B Charette, 2007-09). He completed a total synthesis of antifungal bixosazole natural product Bengazole A (with Professor Steven V Ley CBE FRS FMedSci, 2003-06). He has also spent time working in medicinal chemistry in the pharmaceutical industry.
Dr Oscar Ces (CB)

Dr Oscar Ces is co-supervisor of (a) the Membrane Biophysics Research Group and (b) the Single Cell Proteomics Research Groups and co-director of (c) Chembecell Ltd and (d) the Non-Specific Binding Initiative (in collaboration with GSK plc). His principal research interests are concerned with studying the mechanics of biological membranes and translating this knowledge base to make technological advances in the fields of drug-membrane and protein-membrane interactions and single cell proteomics. To remain at the forefront in the area of biomembrane research he has an ongoing programme of novel equipment development including specialist X-ray beamlines and microfluidic platforms for single cell proteomic studies.

The Membrane Biophysics group, run jointly with Professor Richard Templer, Professor John Seddon and Dr Rob Law has recently embarked on a £1.75M EPSRC funded platform grant centred around core themes including the role of bilayer asymmetry in regulating biological function and protein control of lipid morphology. Established research programmes within this group include looking at the effect of the inositol phospholipids and their different phosphorylation states on stored elastic stresses and hence the activity of related kinases and phosphatases (with Dr Piers Gaffney and Dr Rudiger Woscholski, Imperial College London). With Professor Shamshad Cockcroft (University College London) and Professor Miguel Seabra (Imperial College London) the group is studying how the biomechanical properties of lipid bilayers regulate the function of phosphatidylinositol transfer proteins (PITPs) and RAB proteins respectively. Alongside Dr Rudiger Woscholski (Imperial College London) his group is studying the acid chain sensitivity of the type II 5-phosphatases and the mechanisms behind SNARE protein driven membrane fusion events (with Professor Paul Freemont, Dept of Biological Sciences, Imperial College London) using biomechanical microscopes incorporating micropipette aspiration platforms.

Most recently the group has been commissioned to design and construct a time resolved millisecond pressure jump X-ray cell that will be based at beamline I22 at Diamond as a user facility. This platform will allow experimentalists to probe the time-dependent structural behaviour of a wide variety out-of-equilibrium soft condensed matter systems and will be online in October 2009.

The Non-Specific Binding Initiative is a £1M multi-disciplinary project aimed at studying the role played by biological membranes in regulating the behaviour of drug molecules in-vivo. Since its inception this research team has identified for the first time that CADs (Cationic Amphiphilic Drugs), the largest class of commercially available drug catalyze a reaction that degrades the phospholipid fabric of plasma membranes. They do not interact passively with cellular membranes as postulated by current drug translocation mechanisms. This phenomenon and its link to a variety of key biological processes is now being studied in collaboration with GSK plc (Clinical Imaging Centre, Hammersmith, London).

The Single Cell Proteomics (SCP) Group is a £5M multidisciplinary initiative funded by the EPSRC to create an advanced suite of technologies for the study of single cells using proteomic approaches. The project includes teams from Imperial, the Institute of Cancer Research and the London Research Institute of Cancer Research UK. In 2008 the SCP project successfully completed its mid-term review. An example of one of the technologies developed as part of this initiative is that of nanodigestion, a wholly unique new platform for the spatially selective digestion of single cells using Smart Droplet Microtools (SDMs). During nanodigestion, spatially selective membrane digestion is effected using optically trapped micron sized oil droplets (SDMs) coated with a variety of amphiphilic monolayers that are brought into controlled contact with target cells in microfluidic environments.

Most recently he has commenced a £250k EPSRC funded Feasibility Account Bid looking at making vesicle machines.

2009 Publications

Peiro-Salvador T, Ces O, Temple RH and Seddon AM

**Buffers May Adversely Affect Model Lipid Membranes: A Cautionary Tale**

Biochemistry, (2009), DOI: 10.1021/bi0901646

Shearman GC, Ces O and Templer RH

**Towards an understanding of phase transitions between inverse bicontinuous cubic lyotropic liquid crystalline phases**


**Droplet-Based Compartmentalization of Chemically Separated Components for Two-Dimensional Separations**

Chem. Commun., (2009), 6159-6161

Seddon AM, Casey D, Stanley CE, Templer RH, and Ces O

**Drug interactions with lipid membranes**

Chem Soc Rev, 38, (2009), 2509-2519, DOI: 10.1039/b813853ms,


**A Microfluidic Platform for Probing Single Cell Plasma Membranes Using Optically Trapped Smart Droplet Microtools (SDMs)**

Lab Chip, DOI: 10.1039/b816657a (2009)


**The lyotropic phase behaviour of ester quaternary surfactants**

J Colloid Interface Sci, 311, (2009), 461-469


**Factors controlling the stability of a kinetically hindered lamellar-lamellar transition**


Shearman GC, Tyler AI, Brooks NJ, Templer RH, Ces O, Law RV and Seddon JM

**A 3-D hexagonal inverse micellar lyotropic phase**


Gauthé BLLE, Heron AI, Seddon JM, Ces O and Templer RH

**Novel osmotic cell for the study of lyotropic systems using X-ray diffraction**

Rev Sci Instrum, 80, (2009), 035107-035107
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.

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.

2009 Publications

Carballares S, Craig D, Hyland CJT, Lu P, Mathie T and White AJP
Highly regioselective ring-opening of trisubstituted aziridines by sulfur-stabilised carbanions

Camp JE and Craig D
Reactivity of dearamatised furans synthesised via the decarboxylative Claisen rearrangement
Tetrahedron Lett. 2009, 50, 3503-3508

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-Organo 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 7Li,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.
2009 Publications

Bompolarla R, Davies RP, Hornauer S and White AJP
The influence of tetrahydrofuran on the structures and reactivities of lithium organo-amidocuprates
Dalton Trans., 2009, 1104-1106

Bompolarla R, Davies RP, Gray T and White AJP
Synthesis of Lithium Ferrocenylcuprates and Their Oxidative Coupling Reactions
Organometallics, 2009, 28, 4632-4635

Crabb E, Davies RP, Janes R, Moore E, Smart L and Walton P
Metals and Life

Professor Andrew de Mello (NMD)
Professor Andrew de Mello’s research group is engaged in a broad range of activities in the general area of microfluidics and nanoscale science. Primary specialisations include the development of microfluidic devices for analytical and bioanalytical applications, ultra-sensitive optical detection techniques, nanofluidic reaction systems for chemical synthesis, novel methods for nanoparticle synthesis and the exploitation of semiconducting materials in diagnostic applications. He has been a member of the Department of Chemistry at Imperial since 1997 and now holds the Chair of Chemical Nanosciences and is Head of Nanostructured Materials and Devices Group. In 2002 he was awarded the SAC Silver Medal by the Royal Society of Chemistry for his contributions to the Analytical Sciences, in 2004 became a Fellow of the Royal Society of Chemistry and in 2008 was awarded the Clifford Paterson Lectureship and Medal by the Royal Society for his contributions to Engineering and Nanotechnology.

2009 Publications

Srisa-Art M, deMello AJ, Edel JB
High-throughput confinement and detection of single DNA molecules in aqueous microdroplets
Chem Commun, 2009, 6548-6550

Chan KLA, Gulati S, Edel JB et al
Chemical imaging of microfluidic flows using ATR-FTIR spectroscopy
Lab Chip, 2009, 9, 2909-2913

Removal of background signals from fluorescence thermometry measurements in PDMS microchannels using fluorescence lifetime imaging
Lab Chip, 2009, 9, 3437-3441

Srisa-Art M, Bonzani IC, Williams A, Stevens MM, deMello AJ and Edel JB
Identification of Rare Progenitor Cells from Human Periosteal Tissue using Droplet Microfluidics
Analyst, 2009, 134, 2239-2245

Hong J, Choi M, deMello AJ and Edel JB
Interfacial Tension-Mediated Droplet Fusion in Rectangular Microchannels

Droplet-Based Compartmentalization of Chemically Separated Components in Two-Dimensional Separations
Chemical Communications, 2009, 6159-6161

Niu XZ, Gielen F, deMello AJ and Edel JB
Electro-Coalescence of Digitally Controlled Droplets
Analytical Chemistry, 2009, 81, 7321-7325

Miller P, Long N, Vilar R et al
Novel Microreactor Technologies for 11C Radiolabelling
Journal of Labelled Compounds and Radiopharmaceuticals 2009, 52, S13-S13

deMello AJ and Wootton RCR
Miniaturisation: Chemistry at the Crossroads
Nature Chemistry, 2009, 1, 28-29

Wang G, Lim C, Chen L et al
Surface-enhanced Raman scattering in nanoliter droplets: towards high-sensitivity detection of mercury (II) ions
Analytical Bioanalytical Chemistry, 2009, 394, 1827-1832

Pereira F, Hassard S, Hassard J and deMello AJ
CE of dsDNA in low-molecular-weight polyethylene oxide solutions
Electrophoresis, 2009, 30, 2100-2109

Gulati S, Rouilly V, Niu XZ et al
Opportunities for microfluidic technologies in synthetic biology
Journal Royal Society Interface, 2009, 6, 1742-5689

Srisa-Art M, Kang DK, Hong J et al
Analysis of protein-protein interactions by using droplet-based microfluidics

Hong J, Paik H, Hwang H et al
The effect of growth temperature on physical properties of heavily doped ZnO:Al films

Wang KH, Amatatongchai M, Nacapracha D et al
Thin-film organic photodiodes for integrated on-chip chemiluminescence detection – application to antioxidant capacity screening
Sensors and Actuators B: Chemical, 2009, 140, 643-648

Lanigan PMP, Ninkovic T, Chan K et al
A microfluidic platform for probing single cell plasma membranes using optically trapped Smart Droplet Microtools
Lab Chip, 2009, 9, 1096-1101

 Huebner A, Bratton D, Whyte G et al
Static microdroplet arrays: a microfluidic device for droplet trapping, incubation and release for enzymatic and cell-based assays
Lab Chip, 2009, 9, 692-698

Hong J, Edel JB and deMello AJ
Micro- and nanofluidic systems for high-throughput biological screening
Drug Discovery Today, 2009, 14, 134-146

Gielen F, deMello AJ, Cass T et al
Increasing the Trapping Efficiency of Particles in Microfluidic Planar Platforms by Means of Negative Dielectrophoresis

Schaerli Y, Wootton RC, Robinson T et al
Continuous-Flow Polymerase Chain Reaction of Single-Copy DNA in Microfluidic Microtools
Analytical Chemistry, 2009, 81, 302-306
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.

**2009 Publications**


Wang XH, Amatongchail M, Nacapricha D, Hofmann O, de Mello JC, Bradley DDC and de Mello AJ

*Sensor Actuat B-Chem., 2009, Vol:140, Pages:643-648, ISSN:0925-4005*

Jin R, Levermore PA, Huang J, Wang X, Bradley D and de Mello JC


Gather MC, Jin R, de Mello JC, Bradley DDC and Meerholz K


Rogel-Salazar J, Bradley DD, Cash JR and de Mello JC


Huang J and de Mello JC

**Dr 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 and the Korea Advanced Nanofabrication Centre. Singapore, GeorgiaTech in Atlanta USA, Ajou University in Korea include the Institute of Materials Research and Engineering in cost sensors for point-of-care diagnostics; other collaborations Imperial spin-out company specializing in the development of low

In recent years, Dr Díez-González’s research has concentrated on the preparation and application in catalysis of N-heterocyclic carbene-bearing complexes in catalysis. Studies have been made of palladium, nickel, gold and ruthenium systems, eventually focussing on organocopper chemistry. The objective of her work is to develop novel families of complexes, active in catalysis, while unveiling their activation/reactivity modes. The ultimate goal is to identify more performing catalysts, better synthetic approaches and a deeper understanding of the reaction pathways.

At present, her research themes are getting broader, as the systems under study are no longer restricted to a sole metal or ligand family. The common link remains the use of pre-formed catalyst whenever possible as her philosophy is to consider them as a tool for bringing some light in the so-called blackbox of catalysis. Hence, well-defined systems allow for a strict control of the ligand/metal ratio and binding mode, which make us closer to the nature of the catalytically relevant species in the reaction media. The transformations currently being examined include cycloaddition (and Click chemistry in particular), cross-coupling and C–H activation reactions.

**2009 Publications**


Levermore PA, Jin R, Wang XH, de Mello JC and Bradley DDC

ADV. FUNCT. MATER., 2009, Vol:19, Pages:950-957, ISSN:1616-301X

Gather MC, Jin R, de Mello JC, Bradley DDC and Meerholz K

APPL. PHYS. B-LASERS O, 2009, Vol:95, Pages:113-124, ISSN:0946-2171

Rogel-Salazar J, Bradley DD, Cash JR and de Mello JC


Huang J and de Mello JC

**Dr Silvia Díez-González (CAM)**

Dr Silvia Díez-González is an Imperial Junior Research Fellow. Educated as an organic chemist, her main research interest resides in the development of novel well-defined organometallic species and their use in organic reactions, specifically carbon–carbon or carbon–heteroatom bond forming reactions.

In recent years, Dr Díez-González’s research has concentrated on the preparation and application in catalysis of N-heterocyclic carbene-bearing complexes in catalysis. Studies have been made of palladium, nickel, gold and ruthenium systems, eventually focusing on organocopper chemistry. The objective of her work is to develop novel families of complexes, active in catalysis, while unveiling their activation/reactivity modes. The ultimate goal is to identify more performing catalysts, better synthetic approaches and a deeper understanding of the reaction pathways.

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**2009 Publications**


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APPL. PHYS. B-LASERS O, 2009, Vol:95, Pages:113-124, ISSN:0946-2171

Rogel-Salazar J, Bradley DD, Cash JR and de Mello JC


Huang J and de Mello JC

**Professor James Durrant (NMD)**

The development of renewable, low cost energy technologies is now widely considered to be a key scientific challenge for the 21st century. The Durrant group’s primary research interest is the development of new chemical approaches to 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 co-ordinating research activities across the College through his position as Deputy Director of Imperial’s Energy Futures Lab, Co-ordinator of Imperial’s Solar Network and Deputy Director of the Doctoral Training Centre in Plastic Electronics.

2009 Publications

Clarke TM, Jamieson FC and Durrant JR
Transient Absorption Studies of Bimolecular Recombination Dynamics in Polythiophene: Fullerene Blend Films

Bredds JL and Durrant JR
Organic Photovoltaics

Benson-Smith JJ, Ohkita H, Cook S, Durrant JR, Bradley DDC and Nelson J
Charge separation and fullerene triplet formation in blend films of polyfluorene polymers with [6,6]-phenyl C61 butyric acid methyl ester
Dalton Transactions, 2009, 10000-10005

Barnes PRF, Liu LX, Li XE, Anderson AY, Kissenerwan H, Ghaddar TH, Durrant JR and O’Regan BC

Distorted Asymmetric Cubic Nanostructure of Soluble Fullerene Crystals in Efficient Polymer: Fullerene Solar Cells

O’Regan BC and Durrant JR
Kinetic and energetic paradigms for dye-sensitized solar cells: moving from the ideal to the real

Charge photogeneration in polythiophene-perylene diimide blend films
Chemical Communications, 2009, 5445-5447

Morandeira A, Lopez-Duarte I, O’Regan B, Martinez-Diaz MV, Forneli A, Palomares E, Torres T and Durrant JR
Ru(II)-phthalocyanine sensitized solar cells: the influence of co-adsorbents upon interfacial electron transfer kinetics

Atienzar P, Ishwara T, Horie M, Durrant JR and Nelson J
Hybrid polymer-metal oxide solar cells by in situ chemical polymerization

Astuti Y, Topoglidis E, Cass AG and Durrant JR
Direct spectroelectrochemistry of peroxidases immobilized on mesoporous metal oxide electrodes: Towards reagentless hydrogen peroxide sensing

Kemp GL, Marritt SJ, Li XE, Durrant JR, Cheesman MR and Butt JN
Opportunities for mesoporous nanocrystalline SnO2 electrodes in kinetic and catalytic analyses of redox proteins
Biochemical Society Transactions, 2009, Vol:37, 368-372


McCall KL, Jennings JR, Wang HX, Morandeira A, Peter LM, Durrant JR, Yellowlees LJ, Woollins JD and Robertson N
Novel ruthenium bipyridyl dyes with S-donor ligands and their application in dye-sensitized solar cells

Koops SE, O’Regan BC, Barnes PR and Durrant JR
Parameters influencing the efficiency of electron injection in dye-sensitized solar cells

Barnes PRF, Anderson AY, Koops SE, Durrant JR and O’Regan BC
Electron Injection Efficiency and Diffusion Length in Dye-Sensitized Solar Cells Derived from Incident Photon Conversion Efficiency Measurements

Dr Joshua Edel (CP)

Dr Josh Edel has a strong track record in the area of nanobiotechnology with primary specializations that include the development of micro and nanofluidic devices for analytical and bio-analytical applications, and ultra-high sensitivity optical detection techniques. His 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. Key achievements include developing novel spectroscopic approaches utilizing the added benefits of nanofluidics to maximize molecular detection efficiencies. For example, a high spatial resolution method utilizing Zero Mode Waveguides (ZMW) was developed to monitor single molecule dynamics in living cells. ZMW were used to confine fluorescent excitation to approximately a 100 nm region of the cellular membrane to monitor lipid diffusion. As another example, Dr Edel has developed technology incorporating novel bioengineered DNA nano-barcodes and nanofluidic channels for performing single molecule biological assays. The described system responds with enough speed and precision to detect 99 percent of all molecules flowing through the detection probe volume and expertise in this area is invaluable with respect to the current application.
In contrast with the established silicon solar cells, organic solar cells have steadily improved over the past few years and the leading device efficiencies are now around 7%. The solar-to-electric power conversion efficiencies of more economical materials like plastics, called organic solar cells, have never been demonstrated with organic solar cells. Most of the research published on organic solar cells is concerned only with increasing the efficiency; device lifetimes are typically not investigated at all. This is quite misleading for the unenlightened reader but not at all surprising given that lifetimes may be only hours when outside of a protective atmosphere or a few weeks for a sealed device. Yet even a low-efficiency organic solar cell will find a market if it is both inexpensive and stable, whereas one boasting an impressive initial efficiency but a ‘supermarket shelf life’ is simply not commercially viable. In contrast with organic solar cells, silicon solar cells have device lifetimes of greater than 20 years outdoors.

### 2009 Publications

**Dr Matthew J Fuchter (Synthesis)**

Dr Matthew Fuchter is a Lecturer in Synthetic and Medicinal Chemistry, as well as a Project Manager within the Drug Discovery Centre. Novel, efficient, and effective synthesis is key to all aspects of research carried out by his group, and his expertise lies in the development of new synthetic methods, target-based synthesis, and medicinal chemistry towards novel anti-cancer therapeutics.

Previously, he has been instrumental in the development of new synthetic methods and biological applications of the porphyrine macrocycles (in collaboration with Professor A G M Barrett FRS FMedSci). 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 porphyrines, the preparation of polymer-supported photooxygenation catalysts, and the conjugation of phototoxic porphyrine 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 Anti-Cancer 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 in 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 enzymes important in 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.

**Novel chemical methodology**

The development of clean and efficient synthetic procedures is of key interest to the Fuchter Group. They have recently developed a one-pot synthesis of aliphatic chlorides from aldehydes. Importantly this process utilises a mechanistically novel C-O bond fission process. 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 synthetic strategies for the asymmetric synthesis of carbocentric and heterocyclic helicenes, as well as surveying their uses in synthetic chemistry and beyond.

As part of his responsibilities as a Project Manager within the Drug Discovery Centre, Dr Fuchter coordinates a cross-College small molecule cancer drug discovery group, 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.

**2009 Publications**


*"Push-Pull" Tropylium-Fused Aminoporphyrazine*


Goslinski T, Zhong C, Fuchter MJ, White AJP, Barrett AGM and Hoffman BM

*Serendipitous Synthesis of Trimetallic Porphyrazine Triads*


*The development of a highly selective inhibitor of cyclin-dependent kinase 7 (CDK7) which demonstrates anti-tumor activity*

Cancer Res. 2009, 69, 6208

Fuchter MJ, Li JJ and Corey EJE


Fuchter MJ, Li JJ and Corey EJE

*Kumada Cross-Coupling Reaction. In Name Reactions for Homologations Part I; Wiley: New York, March 2009; pp 47-69*

Fuchter MJ, Li JJ and Corey EJE

*Tsuji-Trost Reaction. In Name Reactions for Homologations Part I; Wiley: New York, March 2009; pp 185-211*

Fuchter MJ, Li JJ and Corey EJE


**Professor Susan E Gibson (Synthesis)**

**Application of metal-mediated reactions in organic synthesis**

The Pauson-Khand reaction is a powerful carbon-carbon bond-forming reaction that converts an alkene, an alkyne and carbon monoxide into a cyclopentenone, a useful building block for the synthesis of more complex biologically-active molecules. The reaction has traditionally been mediated by relatively large amounts of a transition metal, however, and although versions that use less metal have been introduced in recent years, these methods still require further development to be truly attractive in an environmentally-aware world. To gain greater insight into the reaction, the Gibson group has been studying an asymmetric catalytic version of the Pauson-Khand reaction using $^{31}$P NMR and X-ray crystallography techniques. This has provided insight into the formation of diastereoisomeric alkyne complexes and their interconversion, and the formation of an unexpected cobalt hydride species during the reaction. Moreover the group is now able to monitor a sub-stoichiometric PKR reaction by $^{31}$P NMR spectroscopy, thus providing a platform for examining the effects of reaction parameters such as temperature and solvent, and the effect of additives. A bisphosphonate enyne, developed to aid the visualisation of the PKR substrate during this work, is proving to be very useful in the study of many more transition metal catalysed cyclisations.

The Gibson group have also designed and executed a new route to synthetically challenging enantiopure tertiary benzyl alcohol. This has been used to achieve the first enantioselective synthesis of gossonorol, a fragrant tertiary alcohol found in many organisms including the cotton plant. Experiments using enantiopure gossonorol are being undertaken to gain insight into the synthesis of other natural products such as the cyclic ether boivinianin B.

Elsewhere in a project designed to discover new fundamental reactivity, the group has discovered that the benzylcarbon of an arane chromium tricarbonyl complex may be deprotonated and the resulting anion oxidised to a species that reacts with oxygen, sulfur and carbon nucleophiles. This represents the first example of the transformation of an benzylc arene chromium tricarbonyl anion to a cation, and its use in bond formation.
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 heterogenous catalysts, where bond formation/breakage and/or electronic effects are important. A prime area of activity is in the construction 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 was later confirmed by experiment. Further work on this protein has also shown that the methodology is capable of being predictive in determining the binding free energies for the native and site-directed mutants. They have been the first group to develop and apply computational chemistry to the problem of assigning 2D-IR spectra of amino-acids and small peptides. This new methodology is very computationally demanding and has required the development of Ab Initio methods to determine the structural relationship to the 2D-IR spectra. One of the group’s aims is to break the timescale barrier in Molecular Dynamics simulations of biological systems. Currently simulations can be routinely applied for 10s of nanoseconds, two orders of magnitude below which interesting chemistry and biology processes occur.

In the next five years the group intends to haul simulations into the microsecond and even millisecond timescale, using massively parallel computers. This will require the development of much more efficient algorithms and computational infrastructure. Concomitant with the development of efficient algorithms to scale up to high processor counts, they will be continually refining our force fields. By the end of the next five years the group aims to routinely run simulations of millisecond duration on systems of greater than a million atoms. In addition they also need to develop fast analytical 3rd derivative codes in Ab Initio quantum chemistry in order to apply and interpret the 2D-IR techniques, mentioned previously, to proteins and other biologically relevant systems. The current computational limitation to the determination and interpretation of the atomic level of detail for the 2D-IR spectra is the calculation of mechanical and electrical anharmonicities. They currently calculate these by numerical differentiation of analytical 2nd derivates using Hartree-Fock or Density Functional Theory based Ab Initio Molecular Orbital methods. This approach 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.

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.
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 CO2 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 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 photophysical processes in organic solar cells.

CURRENT RESEARCH ACTIVITIES INCLUDE:

- The application 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.

Professor Nick Harrison (NMD)

High Surface Area Fluorination Catalysts

Recently high surface area AlF3 has been synthesised and found to catalyse reactions that are usually only catalysed by very strong Lewis acids such as SbF5. This makes it a promising alternate to SbF5 for use as an industrial fluorination catalyst for the production of chloro- and hydrofluorocarbons. Calculations based on density functional theory reveal that the α and β-AlF3 phases expose under-coordinated Al ions that act as Lewis acid sites with the acidity characterised by computed NH3 binding energies and CO vibrational shifts. First principles thermodynamics has been used to predict surface phase diagrams in the presence of water, HCl and HF. There is now a fairly complete understanding of the catalyst composition and structure and the nature of the active sites.

2009 Publications

Leventis HC and Haque SA
Control of charge recombination at nanostructured quantum-dot sensitized TiO2 interfaces employing a multi-step redox cascade
Energy & Environmental Science Volume: 2 Issue: 11 Pages: 1176-1179 Published: 2009

King S, Sommer M, Huettner S et al
Charge separation and recombination in self-organizing nanostructured donor-acceptor block copolymer films
Journal of Materials Chemistry Volume: 19 Issue: 30 Pages: 5436-5441 Published: 2009

Hofmann CC, Bauer P, Haque SA et al
Energy- and charge-transfer processes in flexible organic donor-acceptor dyads
Journal of Chemical Physics Volume: 131 Issue: 14 Article Number: 144512 Published: Oct 14 2009

Tokmoldin N, Griffiths N, Bradley DDC et al
A Hybrid Inorganic-Organic Semiconductor Light-Emitting Diode Using ZrO2 as an Electron-Injection Layer
Advanced Materials Volume: 21 Issue: 34 Pages: 3475–3480 Published: Sep 11 2009

Lee H, Leventis HC, Moon SJ et al
Advanced Functional Materials Volume: 19 Issue: 17 Pages: 2735-2742 Published: Sep 9 2009

Dyer-Smith C, Benson-Smith JJ, Bradley DDC et al
The Effect of Ionization Potential and Film Morphology on Exciplex Formation and Charge Generation in Blends of Polyfluorene Polymers and Silole Derivatives

Wong WW, Jones DJ, Yan C et al
Synthesis, Photophysical, and Device Properties of Novel Dendrimers Based on a Fluorene-Hexabenzocoronene (FHBC) Core
Organic Letters Volume: 11 Issue: 4 Pages: 975-978 Published: Feb 19 2009

Hallett JP, Liotta CL, Ranieri G and Welton T
Charged Nucleophiles: An Ionic Liquid Effect

Charge Screening in the S(N)2 Reaction of Charged Electrophiles and Charged Nucleophiles: An Ionic Liquid Effect

2009 Publications
Long Range Order in Defective Oxides: The Magnelli Phases of TiO$_2$-x

First principles thermodynamics has been used to calculate the equilibrium defect concentration of TiO$_2$ as a function of temperature and oxygen partial pressure. At very low defect concentrations Ti-interstitials are found to be more stable than O-vacancies, at higher concentration the phase diagram contains a sequence of narrow phases with stoichiometries Ti$_{n}$O$_{2n-1}$ with $4 \leq n \leq 9$. These are the Magnelli phases and the computed T,P phase boundaries are in good agreement with those observed.

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.

Carbon Peapod Structures for Spintronics Applications

Sc@C$_{82}$ endohedral fullerenes encapsulated in single walled carbon nanotubes (so called, peapod structures) are a possible realisation of an idealised system of interest for quantum computing i.e. a coupled, one dimensional spin chain. First principles calculations suggest that for either semiconductor or metallic nanotubes the spin resides mainly on the fullerene and that spin interactions decay exponentially with inter-fullerene separation. The system can be described by a Hubbard Anderson model in the limit that U>>t and can therefore be approximated as an ideal antiferromagnetic Heisenberg spin chain.

Additional work includes developing a structural model and a new understanding of the room temperature ferromagnetism in V(TCNE)$_2$, the prediction that ordered defect structures in graphene can produce a room temperature ferromagnet, the characterisation of the gas sensing sites on SnO$_2$ surfaces, the reliable prediction of semiconductor band gaps using hybrid-exchange density functional theory, the development of a new model of inelastic X-ray scattering in Cu$_2$O.

2009 Publications

Pisani L, Montanari B and Harrison NM
*Stability of the ferromagnetic state in a mixed sp(2)-sp(3) carbon system*  
Phys Rev B 80(10) Article number 104415 Sep 2009

Warner JH, Rummel MH, Ge L, Gemming T, Montanari B, Harrison NM, Buchner B and Briggs GAD
*Structural transformations in graphene studied with high spatial and temporal resolution*  

Liborio L, Mallia G and Harrison N
*Electronic structure of the Ti$_4$O$_7$ Magnelli phase*  

Ge L, Jefferson JH, Montanari B, Harrison NM, Pettifor DG and Briggs GAD
*Effects of Doping on Electronic Structure and Correlations in Carbon Peapods*  
Acs Nano 3(5):1069-1076 May 2009

Bailey CL, Mukhopadhyay S, Wander A, Searle BG and Harrison NM
*Structure and Stability of alpha-AlF$_3$ Surfaces*  

De Fusco GC, Pisani L, Montanari B and Harrison NM
*Density functional study of the magnetic coupling in V(TCNE)$_2$*  
Physical Review B 79(8) Article number 085201 Feb 2009

*Electronic structure of Lewis acid sites on high surface area aluminium fluorides: a combined XPS and ab initio investigation*  

Dr Martin Heeney (NMD)

Martin Heeney joined Imperial in May 2009, moving his research groups across London from Queen Mary University of London, where he was a senior lecturer in the Department of Materials. He is an organic materials chemist whose research interests lie in the design, synthesis and characterisation of organic semiconductor materials for a range of optoelectronic applications, including field effect transistors, photovoltaic devices and light emitting diodes. As such, his research is highly multi-disciplinary and collaborative covering aspects of organic, inorganic and polymer chemistry with a central theme of establishing relationships between molecular design, synthetic methodology, processing and performance.

His current research in focused in two main areas, the development of stable semiconductors for field effect transistors and the development of low band gap donor polymer for organic solar cells. In the area of transistor materials, operational and storage stability are critical issues, particularly in devices driven under high current density or operated in a bottom gate configuration where the semiconductor is exposed to the ambient atmosphere. His group is exploring strategies to chemically modify the polymer backbone structure to improve stability, principally by ring fusion with a variety of bridging substituents, leading to changes in both the backbone configuration and microstructure, as well as the electronic energy levels of the molecular orbitals.

Organic solar cells are a potentially promising source of electrical power for portable and off-grid applications due to their combination of low cost, low weight and mechanical flexibility. However current applications are limited by low device efficiencies. Currently some of the best performing devices are based upon donor/acceptor blends of regioregular poly(3-hexyl) thiophene (P3HT) and PCBM respectively. The development of polythiophene analogues that can capture more of the photon flux from the solar spectrum is one strategy to further improve photovoltaic efficiency. This can be achieved by reducing the band gap of the semiconducting polymer. However, an undesirable consequence with this approach can be a reduction in the open circuit voltage of the device (Voc), and therefore a reduction in cell efficiency. The Heeney group are developing a range of semicrystalline selenophene polymers and co-polymers...
for photovoltaic applications. They have demonstrated that certain selenophene polymers exhibit reduced band gaps compared to their thiophene analogues, resulting in enhanced cell photocurrent without a significant loss in open circuit voltage of the photovoltaic device.

2009 Publications

Cates NC, Gyevel R, Beiley Z, Miller CE, Toney MF, Heeney M, McCulloch I, and McGehee MD
Tuning the properties of polymer bulk heterojunction solar cells by adjusting fullerene size to control intercalation
Nanolett, 2009, 9, 4153

Zhao N, Noh Y-Y, Chang J-F, Heeney M, McCulloch I and Sirringhaus H
Polaron localisation at interfaces in high mobility microcrystalline conjugated polymers

Ball JM, Wobkenberg PH, Colleaux F, Heeney M, Anthony JE, McCulloch I, Bradley DDC and Anthopoulos TD
Solution processed low-voltage organic transistors and complementary inverters
Appl. Phys. Lett. 2009, 95, 103310

Rofle NJ, Heeney M, Wyatt PB, Drew Al, Kreouzis T and Gillin WP
Elucidating the role of hyperfine interactions on organic magnetoresistance using deuterated aluminium tris(8-hydroxyquinoline)
Phys. Rev. B. 2009, 80, 241201

Controlling the orientation of terraced nanoscale ‘ribbons’ of a poly(thiophene) semiconductor
ACS Nano 2009, 3, 780-787

Hallam T, Lee M, Zhao N, Nandhakumar I, Kemerink M, Heeney M, McCulloch I and Sirringhaus H
Local charge trapping in conjugated polymers resolved by scanning kelvin probe microscopy

High-performance polymer-small molecule blend organic transistors

Distorted asymmetric cubic nanostructure of soluble fullerene crystals in efficient polymer:fullerene solar cells
ACS Nano, 2009, 3, 2557

Jimison LH, Toney MF, McCulloch I, Heeney M and Salleo A
Charge-transport anisotropy due to grain boundaries in directionally crystallized thin films of regioregular poly(3-hexylthiophene)
Adv. Mater. 2009, 21, 156-168

Doping of conjugated polythiophenes with alkyl silanes

Influence of molecular weight distribution on the gelation of P3HT and its impact on the photovoltaic performance
Macromolecules 2009, 42, 4661-4666

Bimolecular crystals of fullerenes in conjugated polymers and the implications of molecular mixing for solar cells

Shoaei S, An ZS, Zhang X, Barlow S, Marder SR, Duffy W, Heeney M, McCulloch I, Durrant JR
Charge photogeneration in polythiophene-pyrene diiodide blend films
Chem. Comm. 2009, 5445-5447

Systematic improvement in charge carrier mobility of air stable triarylmethane copolymers
J. Am. Chem. Soc. 2009, 131, 10814-10815

Smith J, Hamilton R, Heeney M, de Leeuw DM, Cantatore E, Anthony JE, McCulloch I, Bradley DDC and Anthopoulos TD
High-performance organic integrated circuits based on solution processable polymer-small molecule blends
Appl. Phys. Lett., 2009, 93, 253301

Separate charge transport pathways determined by the time of flight method in bimodal polytriarylamine
J. Appl. Phys., 2009, 105, 013701

Bjorklund N, Lill JO, Rajander J, Osterbacka R, Tierney S, Heeney M, McCulloch I and Colle M
The effects of metal impurities in poly[(2,5-bis(3-decylthiophen-2-yl)thieno[2,3-b]thiophene] on field-effect transistor properties

Solid-state supramolecular organization of polythiophene chains containing thienothiophene units
Adv. Mater., 2009, 21, 1193-1198

Semiconducting thienothiophene copolymers: design, synthesis, morphology, and performance in thin-film organic transistors
Adv. Mater., 2009, 21, 1091-1109

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 include aspects of synthetic, coordination and catalytic chemistry, as well as asymmetric synthesis and mechanistic investigations.

A key focus of her more recent 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 dicatolonic nickel(II) catalysts for highly enantioselective aza-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 group includes 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 hydroalkylation reactions for the construction of biologically relevant O-heterocycles (benzopyrans, cyclic ethers and lactones). Recently, further discoveries have been made of the unique regioselectivity of metal triflate catalysts in intramolecular hydroalkylation reactions, and the first report of a Pd-catalysed enantioselective α-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 flow chemistry for organic synthesis.

2009 Publications
Adrio LA, Quek LS, Taylor JG and Hii KK
Copper-Catalysed Intramolecular O-H Addition to Unactivated Alkenes
Tetrahedron, 2009, 65, 10334-10338

Arbour JL, Rzepa HS, White AJP and Hii KK
Unusual Regiodivergence in Metal-Catalysed Intramolecular Cyclisation of γ-Allenols
Chemical Communications, 2009, 3925-3927

Smith AMR, Billen D and Hii KK
Palladium-Catalysed Enantioselective α-Hydroxylation of α-Ketoesters
Chemical Communications, 2009, 3925-3927

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 ºC), and as a class exhibit unusual physical properties; vanishing vapour pressure, large liquidous 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 led into catalyst development, which are then employed in targeted organic synthesis or polymer production. One project includes the development of calcium catalysts for intramolecular hydroamination that are employed to synthesise pharmaceutically 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 biodegradable polymers (used as packaging, fibres or in medicine where a degradable matrix is required) from renewable resources (corn or sugar beet).

2009 Publications
Heavier Group 2 Metals and Intramolecular Hydroamination: A Computational and Synthetic Assessment
Dr Dong Ku Kang (NMD)

Dr Kang has been actively engaged in the development of micro- and nanofluidic systems to biological application. A variety of photonic technologies for investigating various biological systems is employed. In particular, his group focuses on three specific areas: one is the development of highly sensitive optical detection technique on bio-species in a microfluidic channel. This work involves the development of fluorescence life time and fluorescence resonance transfer (FRET) detections for use in small volume of DNA, proteins and cells using a microfluidic channel. The other topic is the molecular imaging of specific cancer biomarkers in single cells or in the cell lysates or in serum from patents to diagnosis. The final one is the detection of protein-protein interaction and the development of a high throughput screening system for inhibitor of protein-protein interaction using microfluidics to diagnosis and drug discovery. These works involve the development of a high resolution imaging technology of specifically distributed biomarkers in pico-litter sample using confocal fluorescence microscopes.

2009 Publications

Truillon R, Kang DK, Park H, Chang SI and O’Hare D
Angiogenin induces nitric oxide synthesis in endothelial cells through PI-3 and Akt kinases
Biochemistry. 2010 Apr 20;49(15):3282-8

Kang DK, Park H, Kang IC and Chang SI
Antigen-antibody Interactions Using Combination of Protein Nanooarray and Atomic Force Measurement

Role of the surface loop on the structure and biological activity of angiogenin
BMB Rep. 2009 Dec 31;42(12):829-33

Analysis of protein-protein interactions by using droplet-based microfluidics
Chembiochem. 2009 Jul 6;10(10):1605-11

Dickson KA, Kang DK, Kwon YS, Kim JC, Leland PA, Kim BM, Chang SI and Raines RT
Ribonuclease inhibitor regulates neovascularization by human angiogenin
Biochemistry. 2009 May 12;48(18):3804-6

Professor David Klug (CB)

Professor David Klug’s work focuses on chemical and biochemical action mechanisms and leads to the development of new tools and methods for investigating the scientific problems of interest. Single Cell Proteomics and Stochastics of Protein Networks. Platform Technologies for the study of Proteomics and Protein-Protein Interactions. Coherent Two Dimensional Infrared Spectroscopy. Natural and Artificial Solar Energy Conversion.

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, faster and more sensitive tools for the analysis of cellular and sub-cellular proteomes. Professor Klug’s group is looking into both label free analysis approaches via innovative spectroscopies such as 2DIR and also approaches that use fluorescence labelling. These are combined with microfluidic approaches to produce novel tools that are able to reveal completely new information regarding how a cell responds to its environment and which proteins interact with which others and also more about the mechanisms and implications of those interactions.

Coherent Two-Dimensional Infrared Spectroscopy: 2DIR is an optical analogue of 2DNMR, but with many orders of magnitude more sensitivity and femtosecond or picosecond time resolution. As the technique is in its infancy there is still a great deal to be done in terms of improving its capabilities as an experimental tool and in learning how to predict and interpret 2DIR spectra directly from quantum chemical calculations in collaboration with colleagues. Professor Klug and his group have recently shown that the particular version of 2DIR under development in their lab can be used to both detect the formation of molecular complexes, and to determine the geometry of the molecular interaction.

Natural and Artificial Solar Energy Conversion: There is a pressing need for new and better sustainable energy sources due to a combination of climate change, economic development of emerging economies and population growth. Higher plant natural photosynthesis is only 1 per cent efficient, yet algae can achieve efficiencies closer to the theoretical limit of ~6 per cent. This is partly because there is not a great deal of evolutionary pressure for higher plants to be particularly efficient at biomass production. Hydrogen is a potential fuel of the future or a reagent that can be used to make high energy fuels. The group are investigating solar-driven water splitting by photocatalysts as a means of clean and efficient hydrogen production. The group is undertaking detailed mechanistic studies to uncover the engineering rules that underlie limitations in efficiency of metal oxide photocatalysts so that they can be improved by rational design.

2009 Publications

Cowan AJ, Tang JW, Leng WH et al
Water Splitting by Nanocrystalline TiO2 in a Complete Photoelectrochemical Cell Exhibits Efficiencies Limited by Charge Recombination

Niu XZ, Zhang B, Marszałek RT et al
Droplet-based compartmentalization of chemically separated components in two-dimensional separations
Chemical Communications Issue: 41 Pages: 6159-6161 (2009)
The shape of the well is quasi-exponential with a half-width equal to \( \frac{A}{2} \), 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 the 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 perfect mirror. This result opens new perspectives for realization of a new generation of self-assembled electrotuneable 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.

2009 Publications

Flatte ME, Kornyshev AA and Urbakh M  
Nanoparticles at electrified liquid-liquid interfaces: new options for electro-optics  

Lee DJ and Kornyshev AA  
Homology recognition funnel  

Kornyshev AA and Wynveen A  
The homology recognition well as an innate property of DNA structure  

Monroe CW, Urbakh M and Kornyshev AA  
Double-Layer Effects in Electrowetting with Two Conductive Liquids  

Kowalski K, Long NJ, Kuimova MK, Kornyshev AA, Taylor AG and White AJP  
Synthesis and characterisation of substituted diphenylamines-charge-transfer, donor-acceptor systems localised at water-oil interfaces  

Kornyshev AA and Spohr E  
Proton transport in polymer electrolyte membranes using theory and classical molecular dynamics, in Device and Materials Modelling in Fuel Cells  

Kornyshev AA  
How physics can inspire biology  
Phys. World 22, 16-17, July (2009)

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.

2009 Publications

Brown RJC, Brett DJL and Kucernak A  
An electrochemical quartz crystal microbalance study of platinum phthalocyanine thin films  
J Electroanal Chem 633(2) 15 Aug 2009

Jiang JH and Kucernak A  
Probing anodic reaction kinetics and interfacial mass transport of a direct formic acid fuel cell using a nanostructured palladium-gold alloy microelectrode  
Electrochim Acta 54(19) 30 Jul 2009
Singlet oxygen work is conducted in collaboration with the group of Professor Peter Ogilby (Aarhus, Denmark). These studies can provide an interesting insight into diffusion processes in live cells, complementary to molecular rotor work described above. This work is concerned with monitoring the cellular distribution and reaction rates of the most important cytotoxic PDT species, singlet oxygen, in single live cells. In PDT, where light induced damage can be precisely localised to a focal point of the pulsed laser, thus TPE PDT can benefit from a focussing lens. TPE PDT should be minimised.

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.

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

**Prizes**

SET for Britain Roscoe Medal for Chemistry and Westminster Medal

**2009 Publications**


**Dr Marina Kuimova (CP)**

Marina Kuimova's research is funded by the EPSRC Life Science Interface 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 rotor work described above. Singlet oxygen work is conducted in collaboration with the group of Professor Peter Ogilby (Aarhus, Denmark).

**Prizes**

SET for Britain Roscoe Medal for Chemistry and Westminster Medal

**2009 Publications**

liquid ordered phase (L_α) phase – present in the fluid (L_α) 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 L_α 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 rigours biophysical determinations of the structure of lipid rafts and exactly what the relationship of lipid rafts is to the L_α 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 L_α phase in the presence of the L_β 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 membrane models it is possible to more accurately determine the role of cholesterol and how it contributes to the formation of the L_α 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 L_α 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 fluorapatite, 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 stipulates 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.

2009 Publications

Seddon AM, Casey D, Law RV, Gee A, Templer RH and Ces O
Drug interactions with lipid membranes

Brauer DS, Karpukhina N, Law RV and Hill RG
Structure of fluoride-containing bioactive glasses
J. Mater Chem., 2009, 19, 5629-5636

O’Donnell MD, Watts SJ, Hill RG and Law RV
The effect of phosphate content on the bioactivity of soda-lime-phosphosilicate glasses

Hill RG, Law RV, O’Donnell MD, Hawes J, Bubb NL, Wood DJ, Miller CA, Mirsaneh M and Reaney I
Characterisation of fluoro containing glasses and glass-ceramics by F-19 magic angle spinning nuclear magnetic resonance spectroscopy

Zainuddin N, Karpukhina N, Hill RG and Law RV
A long-term study on the setting reaction of glass ionomer cements by Al-27 MAS-NMR spectroscopy

Clarke JA, Seddon JM and Law RV
Cholesterol containing model membranes studied by multinuclear solid state NMR spectroscopy
The gas-phase structures of Si₁₀O₁₅H₁₀ (above left), and the D₄ symmetry conformer of Si₆O₁₂Ph₈ (above right).

(Red atoms are oxygen, yellow or blue are silicon, black are carbon, and white, hydrogen.)
Metal-Organic Frameworks for Gas Storage

We extended our work in this area in 2009 and continued to work in collaboration with Dr R Davies and to be funded via the UK Energy Research Centre. 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 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 Drs D Book and A Walton (University of Birmingham).

A metal organic framework based on manganese(II) centres linked by an imidazole-based linker. (Red atoms oxygen, blue nitrogen, green manganese and black carbon, hydrogen atoms omitted.)

2009 Publications

Cordes D, Gazard S and Lickiss P
Superstores
The Chemical Engineer, 2009, 817/8, pages: 34-35

Wann DA, Rataboul F, Reilly AM, Robertson HE, Lickiss PD and Rankin DWH
The gas-phase structure of the decasilsesquioxane Si10O15H10

Ning B, Graham NID and Lickiss PD
A Comparison of Ultrasound based AOPs for the Removal of X-ray Contrast Media Contaminants
Water Science and Technology, 2009, 60, pages: 2383-2390

Wann DA, Reilly AM, Rataboul F, Lickiss PD and Rankin DWH
The gas-phase structure of the hexasilsesquioxane Si6O9(OSiMe3)6
Zeitschrift fur Naturforschung Teil B, 2009, 64B, pages: 1269-1275

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.

Metallocene 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 polymerisation 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 dicationic 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 11C 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 thioesters, forming new transition metal macrocyclic CO/C02-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 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 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 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 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 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 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 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 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 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 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 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 CO2-containing compounds, and applying the syntheses on a microfluidic scale via ‘lab-on-a-chip’ technology. For the first
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.

Dr Ruth Martinez-Casado
(NMD)

Quantum-mechanical studies of atomic helium scattered off metal-oxide surfaces

He-atom scattering from surfaces is nowadays a well-established and valuable tool to characterize the structure of periodic surfaces, to determine gas-surface interaction potentials, or to investigate the presence of defects and adsorbates. Unlike other techniques (e.g., STM or FIM), He-atom scattering causes no damage to the surface, is very surface sensitive as it only probes the outermost layers and does not suffer from the surface charging effects present in other techniques, such as spectroscopy and electron diffraction. However, the correct interpretation and quantitative analysis of the experimental results requires a quantum treatment of both the He-surface interaction potential and the He-atom dynamics. A first-principle description has not previously been possible because the dominant methodology to deal with extended systems is based on density functional theory (DFT), Hartree-Fock (HF) and/or hybrid DFT/HF approaches, which do not describe the dispersion forces correctly, though they dominate the long-range interaction. Dr Ruth Martinez-Casado, Dr Giuseppe Mallia and Professor Nicholas Harrison are currently demonstrating that a realistic description of the He-surface interaction potential can be obtained by using and/or implementing, post-HF-based ab-initio techniques. The aim of this project is to combine this kind of ab-initio methodology with dynamical methods, such as the close-coupling (CC) method, to provide a complete analysis and understanding of He-surface scattering.

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 thiophene 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.

2009 Publications

Miller PW, Jennings LE, de Mello AJ, Gee AD, Long NJ and Vilar R
A microfluidic approach to the rapid screening of palladium-catalysed aminocarbonylation reactions

Jennings LE and Long NJ
‘Two is better than one’ — probes for dual-modality molecular imaging

Kealey S, Long NJ, Miller PW, Plisson C, Martarello L and Gee AD
Copper(I) scorpionate complexes and their application in palladium-mediated [[11]C] carbonylation reactions
Chem. Commun., 2009, pages 3696-698

Long NJ
Dual-modality probes for molecular imaging

Miller PW, Long NJ and White AJ
Synthesis, characterisation and coordination chemistry of a new multidentate P2N4 ligand system
Dalton Trans., 2009, 5284-5286

Synthesis and characterisation of substituted diphenylamines charge-transfer acceptor systems localised at water-oil interfaces
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.

2009 Publications

Zhao N, Noh Y, Chang JF, Heeney M, McCulloch I and Sirringhaus H
Polaron Localization at Interfaces in High-Mobility Microcrystalline Conjugated Polymers
Advanced Materials 21 (2009) 3759-3763

Systematic Improvement in Charge Carrier Mobility of Air Stable Triarylmethine Copolymers

Smith J, Hamilton R, McCulloch I, Heeney M, Anthony JE, Bradley DDC, and Anthopoulos TD
High mobility p-channel organic field effect transistors on flexible substrates using a polymer-small molecule blend

Charge photogeneration in polythiophene-polyene diimide blend films

Bimolecular crystals and intercalated molecular structures of polymer/fullerene in bulk heterojunction solar cells

Semiconducting thienothiophene copolymers: design, synthesis, morphology, and performance in thin-film organic transistors

Bimolecular crystals of fullerenes in conjugated polymers and the implications of molecular mixing for solar cells

Influence of Molecular Weight Distribution on the Gelation of P3HT and Its Impact on the Photovoltaic Performance
Macromolecules (Washington, DC, U.S.) 42 (2009) 4661-4666

Distorted asymmetric cubic nanocrystalline of soluble fullerene crystals in efficient polymer/fullerene solar cells
ACS Nano 3 (2009) 2557-62

Doping of conjugated polyanilines with alkyl silanes

Jimlison LH, Toney MF, McCulloch I, Heeney M and Salleo A
Charge-Transport Anisotropy Due to Grain Boundaries in Directionally Crystallized Thin Films of Regioregular Poly(3-hexylthiophene)

Conducting formulation, (Merck Patent GmbH, Germany; Konarka Technologies GmbH)
Application: WO, 2009, pp. 33-112

Heeney M, Al-Hashimi M, McCulloch I, Zhang W and Hamilton R
Structural and optoelectronic effects of chalcogen atom manipulation on low bandgap polymers

High-performance polymer-small molecule blend organic transistors

Hallam T, Lee M, Zhao N, Nandhakumar I, Kemerlink M, Heeney M, McCulloch I and Sirringhaus H
Local Charge Trapping in Conjugated Polymers Resolved by Scanning Kelvin Probe Microscopy
Physical Review Letters 103 (2009) 4

Controlling the Orientation of Terraced Nanoscale ‘Ribbons’ of a Poly(thiophene) Semiconductor
ACS Nano 3 (2009) 780-787

Chen HL, Hou J, McCulloch I, Raupp GB, Subramnian V and Editors
Special Issue on Flexible Electronics and Displays
In: J. Disp. Technol., 2009; 5(6), 2009

Tuning the Properties of Polymer Bulk Heterojunction Solar Cells by Adjusting Fullerene Size to Control Intercalation
Nano Letters 9 (2009) 4153-4157

Intercalation in polymer-molecule blends
Abstract of Papers, 238th ACS National Meeting, Washington, DC, United States, August 16-20, 2009 (2009) PMSE-527

Solid-state supramolecular organization of polythiophene chains containing thienothiophene units

The effects of metal impurities in poly[(2,5-bis(3-decylthiophen-2-yl)]thieno[2,3-b]thiophene] on field-effect transistor properties

Separate charge transport pathways determined by the time of flight method in bimodal polytriarylamine
J. Appl. Phys. 105 (2009) 013701/1-013701/6

Ball JM, Wobkenberg PH, Colleaux F, Heeney M, Anthony JE, McCulloch I, Bradley DDC and Anthopoulos TD
Solution processed low-voltage organic transistors and complementary inverters
Dr Philip Miller (CAM)

Dr Philip Miller is an EPSRC-LSI (Life Sciences Interface) Fellow jointly associated with the Department of Chemistry and the Aarhus University PET centre in Denmark. His research is focused on the development of new and innovative chemical methods for the preparation of carbon-11 based radiolabelled molecules for use in PET (Positron Emission Tomography) imaging. He is specifically focused on the use of transition metal mediated coupling reactions for the insertion of small radioactive molecules such as $^{11}$CO and $^{11}$CH$_3$I into biologically active molecules. In combination with developing new chemical methods he is also exploring the use of glass and ceramic microfluidic reactors as a practical means of enhancing radiolabelling reactions. In addition to developing $^{11}$C labelling chemistry Dr Miller has interests in fundamental coordination chemistry, carbon-carbon bond forming catalytic reactions, solid supported catalysts and mixed nitrogen-phosphorus ligands.

2009 Publications

Miller PW, Jennings LE, deMello AJ, Gee AD, Long NJ and Vilar R
*A Microfluidic Approach to the Rapid Screening of Palladium-Catalysed Aminocarbonylation Reactions*

Kealey S, Miller PW, Long NJ, Plisson C, Martarello L and Gee AD
*Copper(I) scorpionate complexes and their application in palladium-mediated [C-11]carbonylation reactions*
Chem. Commun., 2009, 3669-3671

Miller PW, Long NJ and White AJP
*Synthesis, characterisation and coordination chemistry of a new monodentate P2N4 ligand system*
Dalton Trans., 2009, 5284-5286

P. W. Miller
*Radiolabelling with short-lived PET (positron emission tomography) isotopes using microfluidic reactors*

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.

The 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.

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.

2009 Publications

O’Regan BC and Durrant JR
*Kinetic and energetic paradigms for dye-sensitized solar cells: Moving from the ideal to the real*

Barnes PRF, Liu LX, Li X, Anderson AV, Kisserwan H, Ghaddar TH, Durrant JR and O’Regan BC
*Re-evaluation of recombination losses in dye-sensitized cells: The failure of dynamic relaxation methods to correctly predict diffusion length in nanoporous photoelectrodes*
Nano Lett. 2009, 9, 3532-3538

Koops SE, O’Regan BC, Barnes PRF and Durrant JR
*Parameters influencing the efficiency of electron injection in dye-sensitized solar cells*
J. Am. Chem. Soc. 2009, 131, 4808-4818

*Structure, Function Relationships in Dyes for Solar Energy Conversion. A Two Atom Change in Dye Structure and the Mechanism for it’s Effect on Cell Voltage*
J. Am. Chem. Soc. 131, 3541, 2009
Morandeira A, Lopez-Duarte I, O’Regan BC, Martinez-Diaz MV, Forneli A, Palomares E, Torres T and Durrant JR

Ru(ii)-phthalocyanine sensitized solar cells: The influence of co-adsorbents upon interfacial electron transfer kinetics  
J. Mater. Chem. 2009, 19, 5016-5026

Barnes PRF, Anderson AY, Koops SE, Durrant JR and O’Regan BC

Electron injection efficiency and diffusion length in dye-sensitized solar cells derived from incident photon conversion efficiency measurements  

Professor David Phillips OBE (CP)

David Phillips is Emeritus Professor and Senior Research Investigator of the Chemical Physics Section. He is currently President Elect of the Royal Society of Chemistry, to become President in 2010.

David Phillips’ research is conducted in collaboration with Dr Marina Kuimova (EPSRC postdoctoral Fellow), the group of Professor Harry Anderson (Oxford), Dr Mahendra Deonarain (Biochemistry), and the Imperial spin-off company PhotoBiotics. The work is exclusively concerned with photodynamic therapy [PDT] of cancer in which photosensitisers are introduced to cells, or tissue, and then irradiated with red light to excite the molecule, which crosses to a long-lived triplet state. This can transfer energy to molecular oxygen to produce excited singlet oxygen, a potent cytotoxic agent. An additional degree of spatial selectivity in PDT, and much deeper tissue penetration, can be achieved by using two-photon excitation. Novel porphyrin photosensitisers with remarkable non-linear properties have been produced, and their cell uptake, localisation and one and two-photon excited PDT efficiencies explored. These sensitizers have also been used for targeted closure of a single blood vessel in an animal model via two-photon excited PDT. PhotoBiotics is concerned with sensitisers [both novel and commercially available] which are covalently bound to monoclonal antibody fragments, conferring a very high degree of selectivity for tumour cells and tissue compared with free sensitisers.

2009 Publications

Membrane-bound molecular rotors measure viscosity in live cells via fluorescence lifetime imaging
J. Phys. Chem. C, 2009, 113 (27), 11634-11642

Photophysical properties and intracellular imaging of water-soluble porphyrin dimers for two-photon excited photodynamic therapy

One- and two-photon activated phototoxicity of conjugated porphyrin dimers with high two-photon absorption cross-sections
Org. Biomol. Chem., 2009, 7, 897-904

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 where the fundamental physical chemistry of flow and particle diffusion and transport are elucidated. Applications include nanofluidic devices for medical applications, gene therapy, nano-medicine and nano-toxicology.

In 2008 the group, in collaboration with our academic visitor Dr V Sokhan, NPL, solved a long standing problem in nanofluidics, deriving a novel expression connecting the interfacial slip in a nanopore to the pore width [Ref 1]. This expression has been tested using simulation and found to hold for a variety of surfaces (M Groombridge, PhD student, work in progress). A new phenomenon involving the saturation of the slip length and its scaling with Knudsen number was discovered. Using experiment, the group (in collaboration with Dr M Thanou, Kings College) produced the first flow measurements for flow through carbon nanotubes (see figures 1,2,3) and reported significantly enhanced flow for polar/non polar fluids [2]. However these flows were significantly smaller than those reported for nanotubes in the literature. This and related EPSRC funded work will form the basis for patents to be submitted through Imperial Innovations.

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).

2009 Publications

Membrane-bound molecular rotors measure viscosity in live cells via fluorescence lifetime imaging
J. Phys. Chem. C, 2009, 113 (27), 11634-11642

Photophysical properties and intracellular imaging of water-soluble porphyrin dimers for two-photon excited photodynamic therapy

One- and two-photon activated phototoxicity of conjugated porphyrin dimers with high two-photon absorption cross-sections
Org. Biomol. Chem., 2009, 7, 897-904
Work on nanoparticle penetration of model lung surfactant monolayers has made significant progress with new data for penetration modes and times obtained from extensive molecular dynamics simulations of polar/non-polar C60 nanoparticles. This research (with Matt Schneemilch, EPSRC postdoc) was submitted for publication early in 2010 and is ongoing.

Figure 4: polar nanoparticles translocating DPPC monolayers from the vapour to the water phase.

References:
Sokhan V and Quirke N
Slip Coefficients in Nanoscale Pore Flow

Whitby, M, Cagnon L, Thanou M and Quirke N
Enhanced Fluid Flow Through Nanoscale Carbon Pipes
Nano Letters, 8, 2632 (2008)

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Professor Mike Robb (CP)

The quantum chemistry group led by Professor Robb is involved in both in 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 09 program suite (see publications). Our applications work involves photochemistry and photobiology.

2009 Publications
Tokmakchev AM and Robb MA
Efficient Generation of Heisenberg Hamiltonian Matrices for VB Calculations of Potential Energy Surfaces

Zachariasse KA, Druzhinin SI, Galievsky VA, Kovalenko S, Senyushkina TA, Mayer P, Noitetmeyer M, Boggio-Pasqua M and Robb MA
Counterintuitive Absence of an Excited-State Intramolecular Charge Transfer Reaction with 2,4,6-Tricyanoanilines. Experimental and Computational Results

Groenhof G, Schäfer LV, Boggio-Pasqua M and Robb MA
Excited State Dynamics in Biomolecules
Handbook of Molecular Biophysics: Methods and Applications, p 93-134 ISBN: 978-3-527-40702-6 Wiley 2009 (Editor: Henrik G Bohr)
Frisch et al
Gaussian 09 Revision A.02
Asturiol D, Lasorne B, Robb MA and Blancafort L
Photophysics of the pπ,pπ* and nπ,pπ* States of Thymine: MS-CASPT2 Minimum-Energy Paths and CASSCF on-the-Fly Dynamics

Boggio-Pasqua M and Robb MA
Groenhof G
Hydrogen Bonding Controls Excited-State Decay of the Photoactive Yellow Protein Chromophore

Araújo M, Lasorne B, Magalhães AL, Worth GA, Bearpark MJ and Robb MA
The Molecular Dissociation of Formaldehyde at Medium Photoexcitation Energies: a Quantum Chemistry and Direct Quantum Dynamics Study

Nenov A, Kölle P, Robb MA and de Vivie-Riedle R
Beyond the van der Lugt-Oosterhoff model: When the Conical Intersection Seam and the S1 Minimum Energy Path do not Cross

Blancafort L, Lasorne B, Bearpark MJ, Worth GA and Robb MA
Second-order analysis of conical intersections: Applications to photochemistry and photophysics of organic molecules n The Jahn-Teller-Effect

Professor Henry Rzepa (Synthesis)

The topological exploration of Mobius systems continued with the identification of systems exemplifying a new concept of p-density wormholes connecting torus knots and links, and with another article summarizing the current theoretical understanding of such systems. During the year, the subject became known as Molecular topology, and a review is planned on this topic next year.

The computational mechanistic exploration of synthetically important catalytic reactions in collaboration with synthetic groups has identified three separate systems for which the origins of regio and stereo-selectivity have been identified.
The use of high level theories to aid in spectral interpretations was epitomized by the simulation of CD (circular dichroism) spectra and the consequent correction of a long standing mis-assignment of the absolute configuration in a higher-order porphyrin.

The use of other topological descriptors of bonding (AIM and ELF) was the topic of a high profile review in Nature Chemistry on the importance of being bonded.

2009 Publications

Rzepa HS
Wormholes in Chemical Space connecting Torus Knot and Torus Link 
π-electron density topologies

Pinto LFV, Glória PMC, Gomes MJS, Rzepa HS, Prabhakar S and Lobo AM
A Dramatic Effect of Double Bond Configuration in N-Oxy-3-aza Cope Rearrangements - A simple synthesis of functionalised allenes

Rzepa HS
The Chiro-optical properties of a Lemniscular Octaphyrin
Org. Lett., 2009, 11, 3088-3091. DOI: 10.1021/ol901172g

Wannere CS, Rzepa HS, Rinderspacher BC, Paul A, Schaefer III HF, Schleyer PvR and Allan CSM
The geometry and electronic topology of higher-order Möbius charged Annulenes
J. Phys. Chem., 2009, 113, 11619-11629. DOI: 10.1021/jp902176a

Rzepa HS
The distortivity of π-electrons in conjugated Boron rings

Rzepa HS
The importance of being bonded
Nature Chem., 2009, 1, 510-512. DOI: 10.1038/nchem.373

Arbour JL, Rzepa HS, White AJP and Hii KK
Metal-Directed Skeletal Diversity in the Cyclization of γ-Allenols

Bonifácio VDB, González-Bello C, Prabhakar S, Rzepa HS and Lobo AM
Chiral aziridination of olefins using a chiral sulfinamide as the nitrogen source
2009, SynLett, December issue

Dr David Scheschkewitz (Synthesis)

Discrete Unsaturated Clusters and Conjugated Systems based on Silicon

The research interests of Dr Scheschkewitz and his group develop around functional compounds with silicon double bonds. Silicon analogues to vinyl lithiums allow for the transfer of Si=Si building blocks to inorganic and organic substrates. Depending on whether suitably reactive residues are present, this may lead to the preservation or consumption of the heavier alkenyl moieties in the resulting products. We focus on two aspects of the very broad chemistry of these novel reagents: 1) The development of a peripheral reactivity in compounds with silicon-silicon double bonds under preservation of both, the degree of unsaturation and the degree of functionality; 2) the deliberate use of the high reactivity of silicon double bonds for the generation of defined small rings and clusters.

Our interest in the transfer of intact silicon double bonds to organic substrates stems from the pronounced effects of the incorporation of these building blocks on band gap and conformation of π-conjugated systems. These effects can be attributed to the inherently smaller energy required to excite Si-Si-π-bonds compared to the C-C congeners, as well as their considerably higher conformational flexibility. We were able to show that even pronounced deviations from planarity do not adversely affect the efficiency of conjugation of Si=Si bonds mediated by organic linking units. We currently investigate the scope of incorporation of Si=Si bonds into extended organic π-systems as well as the tolerance of functional groups in general and their chemical transformations.

While it is hence often desirable to maintain the integrity of the Si=Si bond, we also systematically exploit the high reactivity of such bonds for the targeted synthesis of homo- and heteronuclear small, silicon-based rings and clusters. These compounds structurally resemble intermediates of gas phase reactions involved in the thermal decomposition of silanes, as well as sub-nanoscalar residues occurring in some forms of bulk elemental silicon (e.g. porous silicon). Our approach enables us to isolate structural motifs, study their molecular and electronic structure, as well as their optical properties.

2009 Publications

Scheschkewitz D
Anionic Reagents with Silicon Containing Double Bonds
Chemistry – A European Journal, 2009, 15, 2476-2485

Abersfelder K, Nguyen T-l and Scheschkewitz D
Stannyl-Substituted Disilenes and a Disilastannirane
Zeitschrift für Anorgansiche und Allgemeine Chemie, 2009, 635, 2093-2098
work was announced in December 2008. With Dr Fernando imaging are under development. New EPSRC funding for this detection of inflammation in myocarditis using ultrasound clinical and non-clinical colleagues, targeted lipid microbubbles

Liquid microbubbles for ultrasound imaging: together with Duncan Bruce at York University, the use of a ruthenium-based

Gokhan Yahioglu. In collaboration with the group of Professor liquid-crystalline phases formed by zinc porphyrin-based crystals, which have potential applications in polymeric sheet polarisers, are being studied. This work was featured on the Fig. 2. 

pressure-jump X-ray apparatus is planned as a further future years (from February 2009).

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).


Lipid membrane microdomains: with Dr Rob Law and Professor Tony Magee (NHLI) the structure and properties of cholesterol-containing model membrane systems are being studied, with a view to their possible roles in various biological functions.

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, lipid 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 Yahioglu. 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

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, phosphorus, and cellulose.

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 and electrodes (capacitors, photovoltaics, fuel cells)
- (Fine structured) carbon nanotube composites, including foams and hybrid systems with conventional carbon fibres

The last century of materials chemistry has proven the enormous value to society of controlling both the composition

2009 Publications

Clarke JA, Seddon JM and Law RV
Cholesterol containing model membranes studied by multinuclear solid state NMR spectroscopy

Shearman GC, Yahioglu G, Kirstein J, Milgrom LR and Seddon JM
Synthesis and phase behaviour of β-octaalkyl porphyrins

Shearman GC, Ugazio S, Soubiran L et al
The lyotropic phase behaviour of ester quaternary surfactants
Journal of Colloid and Interface Science, 2009, 331, pages 463-469

Shearman GC, Tyler A, Brooks NJ et al
A 3-D hexagonal inverse micellar lyotropic phase
Journal of the American Chemical Society, 2009, 131, pages 1678-1679

Shearman GC, Ugazio S, Soubiran L et al
Factors controlling the stability of a kinetically hindered lamellar-lamellar transition

Gauthe BILLE, Heron AJ, Seddon JM et al
A high pressure cell for simultaneous osmotic pressure and X-ray diffraction measurements
Reviews of Scientific Instruments, 2009, 80, pages 035107 - 1 to 10

Squires AM, Conn CE, Seddon JM et al
Quantitative model for the kinetics of lyotropic phase transitions involving changes in monolayer curvature
Soft Matter, 2009, 5, pages 4773-4779

Sagnella SM, Conn CE, Krodkiwksa L et al
Ordered nanostructured amphiphile self-assembly materials from endogenous non-ionic unsaturated monoethanolamide lipids in water
Langmuir, in press

Mohamad-Aghaie D, Mace E, Sennoga CA et al
Molecular dynamics simulations of liquid condensed to liquid expanded transitions in DPPC monolayers
Journal Of Physical Chemistry B, in press

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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. The group is currently exploring new, potentially large volume, synthetic methods produce ever more reliable materials, the next challenge is to assemble them into higher order structures. As a related strategy, the group grows nanotubes onto conventional micron-sized fibres to create hierarchical structures suitable for both structural and multi-functional composites. A new, scalable gas phase approach has been developed to produce large volumes of chemically-modified carbon nanotubes with a minimum of waste; in principle, it 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.

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 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. 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.

2009 Publications

Rahatekar S, Shaffer MSP and Elliott J

Modelling percolation in fibre and sphere mixtures: Routes to more efficient network formation

Comp. Sci Tech., In Press, 2009

Bangarusanpath D, Ruckdaschel H, Altstadt V, Sandler J, Garry D and Shaffer MSP

Rheology and properties of melt-processed poly(ether ether ketone)/multi-wall carbon nanotube composites

Polymer, 50, 24, 5803-5811, 2009

Orchard KL, White AJP, Shaffer MSP and Williams CK

Pentanuclear Complexes for a Series of Alkylzinc Carboxylates

Organometallics, 28, 5828-5832, 2009

Qian H, Greenhalgh E, Bismarck A and Shaffer MSP

Synthesis and characterisation of carbon nanotubes grown on silica fibres by injection CVD


Gonzalez A, Orchard K, Sato N and Williams CK

One-pot, in situ synthesis of Zn2O-carbon nanotube-epoxy resin hybrid nano-composites

Chem. Comm., 4034-4036, 2009

Bangarusanpath D, Ruckdaschel H, Altstadt V, Sandler J, Garry D and Shaffer MSP

Rheological and electrical percolation in melt processed poly(ether ether ketone)/multi-wall carbon nanotube composite


Menzel R, Lee A, Bismarck A and Shaffer MPSI

Inverse Gas Chromatography of as-received and modified carbon nanotubes

Langmuir, 25(14), 8340–8348, 2009

Thomas B, Boccaccini A and Shaffer MSP

Sol-Gel silica nanotube composites


Cho J, Boccaccini A and Shaffer MSP

Ceramic matrix composites containing carbon nanotubes (a review)


Winchester RAL, Whitby M and Shaffer MSP

Synthesis of pure phosphorus nanostructures


Verdejo R, Werner P, Sandler J, Altstädt V and Shaffer MSP

Morphology and properties of injection-moulded carbon-nanofibre poly(etheretherketone) foams


Enhanced damping in flexible polyurethane foams filled with carbon nanotubes


Cho J, Konopka K, Rozniatowski K, Garcia-Lecina E, Shaffer MSP and Boccaccini AR

Characterisation of carbon nanotube films deposited by electrophoretic deposition

Carbon, 47, 58-67, 2009

Verdejo R, Jell G, Safinia L, Stevens M, Bismarck A and Shaffer MSP

Reactive polyurethane carbon nanotube foams and their interactions with osteoblasts

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, evoninic acid, iso-evoninic 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 have are developing a synthesis of asperecyclide 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-FcεRI protein-protein interaction – We have a collaboration with Robin Leatherbarrow (Chemistry, IC), Brian Sutton and Andrew Beavil (Structural Biology, KCL) developing peptide-based antagonists of the above-mentioned protein-protein interaction:

Small molecule regulators of LRH-1 – We have a collaboration with Simak Ali (IC, Oncology Hammersmith) 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 18F labelled HER-1 & HER-1 receptor imaging agents for PET – We have a collaboration with Eric Aboayge (IC, Oncology Hammersmith) developing methods for 18F labeling of certain heterocyclic compounds for imaging of breast cancers:

**2009 Publications**

Spivey AC
*Work Hard, Play Hard – a Work Ethic Forged in the Group Oppolzer*
Chimia 2009, 63, 864–866

Webber MJ and Spivey AC
*Molecular Modelling: Supporting Saytzeff*

Spivey AC, Tseng C-C, Jones TC, Kohler AD and Ellames GJ
*A Method for the Parallel Solid-Phase Synthesis of Iodinated Analogues of the CB1 Receptor Inverse Agonist Rimonabant*
Org. Lett. 2009, 11, 4760-4763

Spivey AC and Arseniyadis S
*Amine, Alcohol and Phosphine Catalysts for Acyl Transfer Reaction*

Spivey AC and Diaper CM
*Silicon and Germanium Linker Units*

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connected chemically, are of interest for drug delivery, oil recovery and to accelerate drug discovery. In the latter case they have continued to produce polymer supports which are more universally applicable to automated drug synthesis. Controlling the formation of gels and their reversible degradation is not only important for drug delivery vehicles but also in aiding the increased challenges in recovering oil from less accessible sources.

They demonstrated that a reductive trigger approach produces polymer gels that can be degraded on demand to unblock, at a desired time, fractured oil containing rock formations (with A. Bismarck, Chem. Eng.). In another collaboration (K. Li, A. Bismarck and A. Livingston, Chem. Eng.) 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.

Conjugated polymers also feature in the collaboration with J. Nelson and D. Bradley (Physics). Here the interest is in understanding the effect of solid-state structure induced through processing on charge mobility. Charge mobility of PPVs with various 2,5-substituted alkoxy sidechains followed the trend of increasing mobility with shorter sidechain lengths.

### 2009 Publications

Tuladhar SM, Sims M, Choulis SA, Nielsen CB, George WN, Steinke JHG, Bradley DDC and Nelson J

**Influence of side chain symmetry on the performance of poly(2,5-diakoxy-p-phenylenevinylene): fullerene blend solar cells**

*Org Electron* 10(4) Jul 2009

Sairam M, Loh XX, Li K, Bismarck A, Steinke JHG and Livingston AG

**Nanoporous asymmetric polyaniline films for filtration of organic solvents**

*J Membrane SCI* 330(1-2) 20 Mar 2009

Loh XX, Sairam M, Bismarck A, Steinke JHG and Livingston AG

**Crosslinked integrally skinned asymmetric polyaniline membranes for use in organic solvents**

*J Membrane SCI* 326(2) 20 Jan 2009


**Influence of alkyl chain length on charge transport in symmetrically substituted poly(2,5-diakoxy-p-phenylenevinylene) polymers**


### 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.

### 2009 Publications

Thongyoo P, Bonomelli C, Leatherbarrow RJ and Tate EW

**Potent inhibitors of β-tryptase and human leukocyte elastase based on the MCoTi-II scaffold**


Wright MH, Heal WP, Mann DJ and Tate EW

**Protein myristoylation in health and disease**


Thomas JC, Green IL, Howson RI, Simpson P, Moss DK, Martin SR, Holder AA, Cota E and Tate EW

**Interaction and dynamics of the Plasmodium falciparum MTIP/MyoA complex, a key component of the invasion motor in the malaria parasite**


Dang THT, de la Riva L, Fagan RP, Heal WP, Janoir C, Fairweather NF and Tate EW

**Chemical probes of surface layer biogenesis in Clostridium difficile**


**N-myristoyl transferase from Leishmania donovani as a Target for Drug Discovery: Structural and Functional Characterisation**


Heal WP and Tate EW

**Getting a chemical handle on protein post-translational modification**

Professor Richard Templer (CB)

Professor Richard Templer holds the Hofmann Chair in Chemistry, is the Director of the Doctoral Training Centre in Chemical Biology (www.chemicalbiology.ac.uk) and the Director of the Porter Alliance for bioenergy research (www.porteralliance.org.uk). His own 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.

This year saw Professor Templer and his colleagues publish papers on the stability of a variety of lyotropic liquid crystal phases. In particular they published a paper on the behaviour of the inverse bicontinuous cubic phases, a long term interest of the group. In addition the membrane biophysics team discovered an entirely new liquid crystalline structure based on a hexagonal packing of spherical micelles and measured the energetics of membrane fusion.

The year saw the graduation of two of Professor Templer’s PhD students, Drs Kulkarni and Turner and the award of a number of grants. The membrane biophysics team received an EPSRC grant to look at the technological challenges of creating vesicle machines – a project commencing in 2010. Professor Templer, representing the Porter Alliance for Biorenewables Research, was one of the members of a pan-European team that were awarded a grant by the European Institute for Innovation and Technology to create a Climate Change Innovation Centre for Europe.

The year also saw Professor Templer, in his role with the Porter Alliance, starting up two companies under the Porter umbrella (Mycologix, a company using fungi to produce biofuel from wood and LCAWorks a company looking at the life cycle sustainability of agricultural and industrial processes), founding the Global Biorenewables Research Society with like minded centres in Europe, the USA, Brazil and Asia, and forging biofuels research alliances with Brazil.

2009 Publications

Peiró-Salvador T, Ces O, Templar RH and Seddon A Buffers may adversely affect model lipid membranes – a cautionary tale Biochemistry 2009, 48, 11149–11151
Shearman GC, Ces O and Templar RH Towards an understanding of phase transitions between inverse bicontinuous cubic lyotropic liquid crystalline phases Soft Matter, 2009
Squires AM, Conn CE, Seddon JM and Templar RH Quantitative model for the kinetics of lyotropic phase transitions involving changes in monolayer curvature Soft Matter, 2009, 5, 4773-4779

Dr Ramon Vilar (CB)

The research in the Vilar Group covers three broad areas: supramolecular, bioinorganic and coordination chemistry. Within these three areas Dr Ramon Vilar’s group aims to understand and use the diverse properties of transition metals (structural, catalytic, optical and magnetic) in a wide range of applications. More specifically:

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 phosphatasess 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.

### 2009 Publications

M. Miller PW, Jennings LE, de Mello AJ, Gee AD, Long NJ & R. Vilar
*A Microfluidic Approach to the Rapid Screening of Palladium-Catalysed Aminocarbonylation Reactions*

B. Barry NPE, Abd Karim NH, Vilar R & Therrien B
*Interaction of ruthenium coordination cubes with DNA*
Dalton Trans. 2009, 10717

O. Owen GR, & Vilar R
*Palladium Iminoacyl Imine Complexes: Strategies towards Imine Insertion Organometallics*, 2009, 29, 5783

S. Suntharalingam K, White AJP & Vilar R
*Synthesis, structural characterisation and quadruplex DNA binding studies of platinum(ii)-terpyridine complexes*
Inorg. Chem. 2009, 48, 9427

V. Vilar R
*Bioinorganic Chemistry*

R. Reed JE, White AJP, Neidle S & Vilar R
*Effect of metal coordination on the interaction of substituted phenanthroline and pyridine ligands with quadruplex DNA*
Dalton Trans. 2009, 2558

C. Mendoza C, Benet-Buchholz J, Pericas M & Vilar R
*Di-platinum complexes containing thiolato-urea ligands: structural and anion binding studies*
Dalton Trans. 2009, 2974

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### 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 anionic nucleophiles to change their reactivity

### 2009 Publications

J. Hallett JR, Liotta CL, Ranieri G & Welton T

E. Correia I & Welton T
*An old reaction in new media: kinetic study of a platinum(ii) substitution reaction in ionic liquids* Dalton Trans., 2009, 4115-4121

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### 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 semiconductors) 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.

**Dr Charlotte Williams (NMD)**

Dr Charlotte Williams researches in the areas of polymer synthesis, catalysis and materials chemistry. She is active in the preparation of metal catalysts (Zn(II), Y(III), Al(III)) for controlled polymerisations, in particular for the ring opening polymerisation of lactide, other lactones and for the sequential copolymerisation of carbon dioxide and heterocycles. Charlotte’s group have studied a series of well defined bis(thio/oxophosphinc amido) yttrium complexes which are very effective catalysts 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.

She is also interested in the synthesis of polymers from renewable resources, e.g. biomass or carbon dioxide and in the preparation of degradable polymers (e.g. aliphatic polyesters, polycarbonates). She has particular interests in the chemistry of polylactide, including its synthesis, properties, applications and degradation. The Williams group have reported a new method to control the stereochemistry of lactide ring opening polymerisation by controlling the nuclearity of the initiator. They have also reported the functionalisation of degradable polymers with carbohydrates. Recently, the Williams group have reported a new carbohydrate lactone, prepared in excellent yield (>90%) from D-glucose. The novel lactone was subsequently polymerised, using a low toxicity zinc catalyst, to produce a functionalised, degradable aliphatic polyester which is highly hydrophilic and can be rapidly degraded to non-toxic, metabolites.

In a third area, she investigates the preparation of new electroactive polymers and organometallic-polymer complexes (iridium complexes) which undergo electroluminescence (emission of light upon application of a voltage) for use as the active layer in polymer light emitting devices. A new class of organometallic iridium complexes which are covalently linked to conjugated polymers and show efficient red light emission have been studied. Finally, the new polymer complexes have emerged as useful tools for understanding the fundamental photophysical processes occurring in polymer solar cells.

In collaboration with Milo Shaffer in the Department of Chemistry, the group have been investigating the preparation of metal oxide nanoparticles from organometallic precursors. This new synthetic route has been demonstrated by the hydrolysis of diethyl zinc, and various heteroleptic alkyl zinc reagents, at room temperature to produce well defined zinc oxide nanoparticles. The synthesis is mild, tolerant and compatible with a range of chemical functional groups, for example we have recently demonstrated the preparation of zinc oxide nanoparticles in epoxy resins systems using this methodology. This enables high loading fractions of well dispersed nanoparticles, in the epoxy resin, to be achieved.

### 2009 Publications

Kember MR, Knight PD, Reung PTR and Williams CK

*Highly Active Dizinc Catalyst for the Copolymerization of Carbon Dioxide and Cyclohexene Oxide at One Atmosphere Pressure*


Tang M, White AJP, Stevens MM and Williams CK

*Biomaterials from Sugars: Polymerisation of a carbohydrate lactone*

Chem. Commun., (2009), 941

Platel RH, White AJP and Williams CK

*Sterecontrolled lactide polymerisation determined by the nuclearity of the yttrium initiator*

Chem. Commun., (2009), 4115

Gonzalez-Campo A, Orchard KL, Sato N, Shaffer M and Williams CK

*One-pot, in situ synthesis of ZnO-carbon nanotube-epoxy resin hybrid nanocomposites*

Chem. Commun., (2009), 4034

Kember MR, White AJP and Williams CK

*Di- and Tri-Zinc Catalysts for the Low-Pressure Copolymerization of CO2 and Cyclohexene Oxide*


Orchard KL, White AJP, Shaffer M and Williams CK

*Pentanuclear Complexes for a Series of Alkylzinc Carboxylates*
systems. The ability to utilise the properties of two or more ligands to link metal centres together in homo- or heteronuclear complexes has been 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, 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.

**2009 Publications**

Lin YH, Leung NH, Holt KB, Thompson AL and Wilton-Ely JDET

*Bimetallic complexes based on carboxylate and xanthate ligands: Synthesis and electrochemical investigations*

Dalton. Trans., 2009, 7829-8128 (Featured on cover and rated as ‘Hot Article’)

Knight ER, Leung NH, Lin YH, Cowley AR, Watkin DJ, Thompson AL, Hogarth G and Wilton-Ely JDET

*Multimetallic arrays: Symmetrical bi-, tri- and tetrametallic complexes*
based on the group 10 metals and the functionalisation of gold nanoparticles with nickel-phosphine surface units
Dalton. Trans., 2009, 3688-3697

Knight ER, Leung NH, Thompson AL, Hogarth G and Wilton-Ely JDET
Multimetallic arrays: Bi-, tri-, tetra- and hexametallic complexes based on gold(I) and gold(III) and the surface functionalisation of gold nanoparticles with transition metals

Hogarth G, Rainford-Brent E-JC-RCR, Kabir SE, Richards I, Wilton-Ely JDET and Zhang Q
Functionalised dithiocarbamate complexes: Synthesis and molecular structures of 2-diethylaminoethyl and 3-dimethylaminopropyl dithiocarbamate complexes

Knight EJ, Cowley AR, Hogarth G and Wilton-Ely JDET
Bifunctional dithiocarbamates: A bridge between coordination chemistry and nanoscale materials
Dalton Trans., 2009, 607-609 (Featured on cover and rated as ‘Hot Article’)

Macgregor MJ, Hogarth G, Thompson AL and Wilton-Ely JDET
Multimetallic arrays: Symmetrical and unsymmetrical bi-, tri- and tetrametallic organometallic complexes of ruthenium(II) and osmium(II)
Organometalics, 2009, 28, 197-208

Dr 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 some times 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.

First general analytical theoretical formulation of the ‘memristor’, the missing circuit element
The experimental realization of the memristor, recently fabricated by the Williams’ group in the Hewlett Packard research labs following on seminal work by Chua in the 70’s, has led to a surge of interest in memristive electronics and their applications. However, a big challenge in the efforts to understand and hence optimally design memristors is the development of a general mathematical framework for its analysis that goes beyond mere computational simulation. Our recently proposed Bernoulli Dynamics framework is a significant step towards this goal. The use of the framework has been demonstrated on the William’s memristor, showing that it constitutes a useful tool suitable for the theoretical analysis, interpretation and evaluation of memristor properties. The value of the Bernoulli formalism lies on the fact that it allows the systematic investigation of a range of memristor properties, such as the hysteretic I-V characteristic curve, by means of explicit analytic relationships which link low-level device parameters with its non-linear dynamics.
### Chemistry

<table>
<thead>
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<th>Class</th>
<th>Title of final year research project</th>
<th>Supervisor</th>
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<tr>
<td>Aldworth, Robin</td>
<td>First</td>
<td>Azahelicenes as organocatalysts</td>
<td>Dr Matt Fuchter</td>
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<tr>
<td>Goh, Astee</td>
<td>First</td>
<td>Synthesis and reactivity of a C2-symmetric enantiopure ether</td>
<td>Professor Sue Gibson</td>
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<td>Hong, Su-Hyun</td>
<td>First</td>
<td>The synthesis of dual modality imaging agents</td>
<td>Professor Tony Barrett</td>
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<td>Juozapavicius,</td>
<td>First</td>
<td>Dye sensitized solar cells</td>
<td>Professor James Durrant</td>
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<td>Koh, Elaine</td>
<td>First</td>
<td>New catalysts for the oxidation of alkanes</td>
<td>Dr George Britovsek</td>
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<td>Lai, Catherine</td>
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<td>Site directed mutagenesis: a key to understanding protein function</td>
<td>Professor Andy Miller</td>
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<td>Chu, Wilton</td>
<td>Upper Second</td>
<td>The capacitance of functionalized metal/liquid interfaces</td>
<td>Dr Tim Albrecht</td>
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<td>Liu, Shan Shan</td>
<td>Upper Second</td>
<td>Approaches to the synthesis of marine natural products</td>
<td>Professor Donald Craig</td>
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<td>Mower, Andrew</td>
<td>Upper Second</td>
<td>Synthesis of novel ionic liquids</td>
<td>Dr Jason Hallett</td>
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<td>See, Hao Jun</td>
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<td>Furanyl glycosides in antibiotic synthesis</td>
<td>Professor Tony Barrett</td>
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<td>Williams, Alexander</td>
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<td>Intramolecular nitrene addition</td>
<td>Dr Piers Gaffney</td>
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<td>Ibrahim, Siti D</td>
<td>Lower Second</td>
<td>Controlling chemistry in molecular-sized reactors (joint with Ed Marshall)</td>
<td>Professor Henry Rzepa</td>
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<td>Ja'Far, Fairuzeta</td>
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<td>Electrically activated synthetic muscles</td>
<td>Professor Anthony Kucernak</td>
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<td>Li, Zhouxiang</td>
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<td>Self assembly of quantum dots at the water-air interface</td>
<td>Dr Fernando Bresme</td>
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<td>Rimington, Emily</td>
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<td>The influence of nanoparticles on electrolyte performance</td>
<td>Professor Milo Shaffer</td>
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<td>Sheppard, Mark</td>
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<td>Designing functional ionic liquids for technological applications</td>
<td>Dr Tricia Hunt</td>
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<td>Hines, Stephen</td>
<td>Third</td>
<td>Synthesis of nitrogen heterocycles by pd catalysis</td>
<td>Dr Mimi Hii</td>
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<td>Strangeways, Jennifer</td>
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<td>The structure of the complex formed between cyamelluric acid and guanadinium picrate: a triangular nanostructure with interesting properties?</td>
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<td>Bailey, Daniel</td>
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<td>Triple stranded DNA molecular dynamics simulations</td>
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<td>Takeichi, Tomohiro</td>
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<td>Helical cation-pl interactions</td>
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### Chemistry and Management

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<td>Ng, Reine</td>
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<td>The Economics of Biofuels</td>
<td>Professor Tony Barrett</td>
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<td>Bakhshi, Kara</td>
<td>Upper Second</td>
<td>The State of Solar Energy</td>
<td>Dr John de Mello</td>
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<td>Cheng, Tze</td>
<td>Upper Second</td>
<td>Interstellar chemistry</td>
<td>Dr Ramon Vilar</td>
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<td>Hale, Zoe</td>
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<td>What Makes a Good Catalyst?</td>
<td>Professor Don Craig</td>
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<td>Jivanj, Sachin</td>
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<td>MMR (measles-mumps-rubella) versus single vaccine jabs</td>
<td>Dr Piers Gaffney</td>
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<td>Lee, Ying</td>
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<td>The processing of chemical waste</td>
<td>Dr Chris Braddock</td>
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<td>Leung, Wanny</td>
<td>Upper Second</td>
<td>The chemistry of coffee</td>
<td>Dr Tim Albrecht</td>
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<td>Sitaram, Varun</td>
<td>Upper Second</td>
<td>The science and economics of drugs used to combat cancer</td>
<td>Professor Sue Gibson</td>
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<td>Yu, Yuan</td>
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<td>Are increased atmospheric CO2 levels really so bad?</td>
<td>Dr Ed Marshall</td>
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<td>Yang, Zhuo</td>
<td>Lower Second</td>
<td>The chemicals involved in Compact and Digital Disks</td>
<td>Professor Henry Rzepa</td>
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### Chemistry with Management

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<td>Cho, Soongwon</td>
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<td>Ultra small voltage driven electrovariable lenses, characterising differential capacitance behaviour in interface between two immiscible electrolytic solution</td>
<td>Professor Alexei Kornyshev, Professor Anthony Kucernak</td>
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<td>Cousens, Nico</td>
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<td>Shape changing liquid droplets</td>
<td>Professor Anthony Kucernak</td>
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<td>Fang, Yue</td>
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<td>Engineering and development of thermo-sensitive nanoparticles for drug delivery using magnetic resonance guided focused ultrasound</td>
<td>Professor Andrew Miller</td>
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<td>Fletcher, James</td>
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<td>Micromechanics of lipid membranes</td>
<td>Professor John Seddon</td>
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<td>Frost, James</td>
<td>First</td>
<td>A cyclopropanation-based approach to seven-membered nitrogen heterocycles</td>
<td>Professor Don Craig</td>
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<td>Huang, Zheng Gang</td>
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<td>Unactivated metal-catalysed couplings</td>
<td>Professor Sue Gibson</td>
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<td>James, David</td>
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<td>Synthesis of low band-gap polymers for organic solar cells</td>
<td>Professor Iain McCulloch</td>
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<td>Jarvis, Robert</td>
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<td>Towards droplet microfluidics for the high throughput screening of PDT sensitisers</td>
<td>Professor Andrew de Mello</td>
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<td>Laraia, Luca</td>
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<td>Synthesis of potential antagonists of nuclear receptors LRH-1</td>
<td>Professor Alan Spivey</td>
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<td>Law, Chun Hung</td>
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<td>Professor James Durrant</td>
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<td>Scadding, Frederick</td>
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<td>Dual MRI-optical probes to image matrix metalloproteinases in vivo</td>
<td>Dr Ramon Vilar</td>
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<td>Shah, Sheena</td>
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<td>Towards point of care cardiac maker testing</td>
<td>Professor Andrew de Mello</td>
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<td>Synthesis of electron rich conjugated polymers for organic electronics</td>
<td>Professor Iain McCulloch</td>
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<td>Scorpionates: flexible ligands for metal coordination</td>
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<td>Photoluminescent liquid crystals</td>
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<td>Alkylation of phenyacetoniitrile in 1-butyl-3-methylimidazolium hydroxide as solvent and catalyst</td>
<td>Dr Jason Hallet</td>
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<td>Dowland, Simon</td>
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<td>Organic light emitting displays</td>
<td>Dr Saif Haque</td>
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<td>Evaluation of novel low bandgap polymers towards higher efficiency organic photovoltaic devices</td>
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<td>Computational modelling of the binding of influenza hemagglutinins to host cells</td>
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<td>Single molecule study of DNA 'telepathy'</td>
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<td>New organocopper compounds for synthetic applications</td>
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<td>Drugs eat membranes</td>
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<td>Deposition of metal nanoparticles of controlled shape</td>
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<td>Revealing regulatory networks controlling photosynthetic efficiency</td>
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<td>Novel lipid based meta-materials</td>
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<td>Ng, Christie</td>
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<td>Making degradable plastics: new tricks for the polycondensation reaction</td>
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<td>Lactide ring-opening polymerisation using Yttrium initiators</td>
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<td>O’Mahony, Flannan</td>
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<td>Quantum dot based nanostructured molecular solar cells</td>
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### Chemistry with Medicinal Chemistry

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<tr>
<td>Li, Mungyuen</td>
<td>First</td>
<td>First Synthesis of beta substituted styrenes by a novel, stereochemically unusual alkenylgermane-aryl bromide cross-coupling reaction</td>
<td>Professor Spivey</td>
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<td>Sun, Lushan</td>
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<td>First Two are better than one: new dual-modality biomedical imaging agents</td>
<td>Dr Nick Long</td>
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<td>Fung, Dorothy</td>
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<td>First The function of lysophospholipids</td>
<td>Dr Rob Law</td>
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<td>Smith, Lucy</td>
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<td>First Blocking protein-protein interactions using structured synthetic peptides—potential anti-allergy agents</td>
<td>Professor Robin Leatherbarrow</td>
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<td>Yau, Hin Chun</td>
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<td>First The role of lipid rafts with drug binding</td>
<td>Dr Rob Law</td>
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<td>Howson, Ronald</td>
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<td>First A novel anti-malarial drug target: throwing a chemical spanner in the plasmodium invasion motor</td>
<td>Dr Ed Tate</td>
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<td>Poon, Elaine</td>
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<td>First Synthetic polymeric receptors for the recognition, separation and identification of phosphoproteins</td>
<td>Dr Joachim Steinke</td>
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<td>Chooi, Kok Phin</td>
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<td>First Asymmetric sigmatropic rearrangement reactions under phase-transfer catalysis</td>
<td>Professor Don Craig</td>
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<tr>
<td>Rose, Kirsten</td>
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<td>First Inhibition of cell-cycle enzymes by metal complexes</td>
<td>Dr Ramon Vilar</td>
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### Chemistry with Medicinal Chemistry and a Year in Industry

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<td>First Oxidation of alkanes: platinum (II) complexes for the oxidation of methane</td>
<td>Dr George Britovsek</td>
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<td>First Developing microfluidic strategies for Scotch whisky authentication</td>
<td>Dr John de Mello</td>
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<td>Gray, Helen</td>
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<td>First New photochemically active polymer materials for intraocular lenses</td>
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### Chemistry with a Year in Industry

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<td>Li, Kim Fung</td>
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<td>Miah, Tanya</td>
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<td>First Metal organic framework with zeolitic structures</td>
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<td>First Towards the biomimetic synthesis of 10-bromo-alpha-chamigrene via an enantiopure bromonium ion</td>
<td>Dr Chris Braddock</td>
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<td>T-e-h, Yih Wei</td>
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<td>First Bio-derived solvents</td>
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<td>First Metal organic frameworks as potential storage media for hydrogen</td>
<td>Dr Paul Lickiss</td>
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### Chemistry with Research Abroad

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<td>Jones, Rachel</td>
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<td>First A radical based approach to primary amines and beta-amino acids</td>
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### Chemistry with Year Abroad

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### Biomedical Physical Chemistry

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<td>Behjat, Hamassaeh</td>
<td>Chemical receptors for phosphatidylinositol phosphates to regulate lipid-protein interactions</td>
<td>Dr Ramon Vilar, Dr Rudiger Woscholski</td>
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<td>Kim, Shinyoung</td>
<td>Development of metal complexes as kinase inhibitors</td>
<td>Dr David Mann, Dr Ramon Vilar</td>
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<td>Lake, Thomas</td>
<td>Investigation into the stable conformations adopted by cyclotide proteins through the use of molecular dynamics simulations</td>
<td>Dr Ian Gould, Professor Robin Leatherbarrow</td>
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<td>Meliga, Stefano</td>
<td>Graph Clustering of Atomic Networks for Protein Dynamics</td>
<td>Dr Mauricio Barahona, Dr Sophia Yaliraki</td>
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<td>Ramji, Kavita</td>
<td>Invading DNA: manipulating transcription factor interactions with novel chemical tools</td>
<td>Dr Ed Tate, Dr Geoff Baldwin, Professor Rob Krams</td>
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<td>Snopek, Martyna</td>
<td>Dynamics of a protein complex involved in the malaria parasite invasion motor</td>
<td>Dr Ed Tate, Dr Ernesto Cota</td>
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### Bioimaging Sciences

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<tr>
<td>Casey, Jonathan</td>
<td>Design of Mixed Lipid Microbubbles for Ultrasound Imaging</td>
<td>Professor John Seddon, Dr Fernando Bresme, Dr Mengxing Tang</td>
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<td>Duffy, Ben</td>
<td>Multimodal Nanoparticles for Image Guided Therapeutics</td>
<td>Dr Maya Thanou, Professor Andy Miller</td>
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<td>Johnson, Helen</td>
<td>Neural Networks for Tumour Detection in PET Dynamic Studies</td>
<td>Dr Subrata Bose, Dr Federico Turkheimer, Professor Eric Aboagye</td>
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<td>Macey, Rosa</td>
<td>Bridging the In-vivo Divide in non-specific binding</td>
<td>Professor Richard Templer, Professor Tony Gee, Professor Nick Long, Dr Oscar Ces, Dr Richard Bazin (Pfizer)</td>
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<td>Sommer, Katherine</td>
<td>Yes WAY! The development of the 5-HT1A receptor radioligand for PET imaging</td>
<td>Dr Philip Miller, Professor Nick Long, Dr Richard Bazin (Pfizer)</td>
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### Chemical Biology of Health and Disease

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<td>Alibhai, Dominic</td>
<td>High throughput FRET of molecular interactions during HIV assembly and budding</td>
<td>Professor Paul French, Professor Mark Neil, Dr Chris Dunsby, Dr Ted Murray (Pfizer), Dr Frank Stuhmeyer (Pfizer)</td>
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<td>Barriga, Hannah</td>
<td>Membrane Protein Refolding</td>
<td>Professor Richard Templer, Professor Paula Booth (Bristol), Dr Oscar Ces, Dr Richard Bazin (Pfizer)</td>
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<td>Bradshaw, Richard</td>
<td>An Integrated Theoretical and Experimental Platform for Probing Protein-Protein Interactions (PPPs)</td>
<td>Dr Ian Gould, Professor Robin Leatherbarrow, Dr Ed Tate, Dr Emmanuelle Caron, Dr Robert Endres</td>
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<td>Koleva, Mirella</td>
<td>Biophysical requirements for Zipper-like phagocytosis</td>
<td>Professor Paul French, Professor Mark Neil, Professor David Carling, Dr Chris Dunsby, Dr Alessandro Sardini</td>
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<td>Laine, Romain</td>
<td>FRET Analysis of Interactions of the Macromolecular Complex AMPK, a Regulator of Cellular Metabolism.</td>
<td>Professor Alan Armstrong, Dr David Mann, Dr Caroline Low</td>
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<td>Single Molecule Measurements of the Catalytic Events in proteolysis</td>
<td>Professor Robin Leatherbarrow, Dr Liming Ying</td>
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<td>Miele, Margherita</td>
<td>Protein-protein interactions in cancer studied using optical analogues of 2D NMR</td>
<td>Professor David Klug, Professor Keith Willison (ICR), Dr Andy Thomas (AstraZeneca)</td>
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<td>Nonoo, Rebecca</td>
<td>Fragment tethering for the development of small molecule inhibitors of protein/protein interactions</td>
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<td>Rosen, Sarah</td>
<td>Modelling mutant receptor-ligand analogue pairs to predict unique phosphoinositide-protein interactions</td>
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<td>Single Molecule Studies on the Allosteric Behaviour of a Protein Folding Nanomachine</td>
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<td>Substrate-directed synthesis of chemical receptors for phosphatidylinositol phosphates to moderate lipid-protein interaction</td>
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<td>Wright, Megan</td>
<td>N-Myristoyl Transferase in Apoptosis and Disease: a Novel Target for Cancer Therapy</td>
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### Green Chemistry

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<td>Supramolecular Approaches For Next Generation Photovoltaic Devices</td>
<td>Dr Joachim Steinke</td>
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<td>Rudaz, Cyrielle</td>
<td>Volatile Methylsiloxanes as Solvents for Synthesis</td>
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<td>Sherwood, James</td>
<td>Conversion of Biomass to Value Chemicals</td>
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<td>Novel Metal Organic Frameworks for the capture of CO2</td>
<td>Dr Rob Davies, Dr Paul Lickiss</td>
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<td>Mechanistic Studies of Organocatalytic Reactions</td>
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<td>Professor Anthony Kucernack, Professor Milo Shaffer</td>
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<td>Transition Metal Catalysts for the Controlled Radical Polymerisation of Vinyl Monomers</td>
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Judy Beard
Director of Development
Imperial College London

Judy Beard joined Imperial as Director of Development in May 2009. Previously she worked for the not-for-profit training and consultancy organisation The Management Centre where she had been Principal Management Consultant since October 2007. Prior to this appointment she worked for 30 years in charities, most recently at Macmillan Cancer Support. During her nine years there she was Director of Fundraising, Marketing and Communications, and in her last six months served as acting Chief Executive Officer. She has previously held senior roles in fundraising at Save the Children, the British Red Cross and the Tate Gallery. She is also a trustee of St Christopher's Hospice in South London.

Simon Bragg
Chief Executive
Oriel Securities

Simon Bragg is Chief Executive and a founder of Oriel Securities Limited, a UK corporate and institutional broker.

Simon graduated in Chemistry from Imperial in 1985. He qualified as a Chartered Accountant with KPMG, before moving to the city where he worked in corporate finance at Hoare Govett. After a spell in private equity, where he founded and headed Cargill’s European Private Equity operations, he moved to HSBC Investment Bank in 1999, before founding Oriel in 2002.

Eileen Boyce
Departmental Operations Manager
Department of Chemistry
Imperial College London

Eileen Boyce joined the Department of Chemistry in November 2007 as the Departmental Operations Manager. Eileen is responsible for the provision of a professional administrative and financial service to support the Department’s teaching and research activities.

Eileen has previously worked for a number of academic institutions in a variety of management roles including Kings College London and Aberdeen University. Eileen holds a BA degree in Philosophy and Geography from University College Cork and an MSc in Information Systems Theory from the University of Westminster.

Anthony Clinch
Senior Advisor
CVC Capital Partners

Tony Clinch is a Senior Advisor to CVC. He has worked in an investment management role in the UK and internationally since 1987. Prior to CVC, he worked in Corporate Banking and Corporate Finance for Citibank in London. A Chartered Engineer, Tony spent his early career with Rolls Royce Ltd. He holds a BSc degree in Engineering and an MSc in Management Sciences from Imperial College London.

Bill Colquhoun
Director
LomondCEOServices LLP

Bill Colquhoun was a Senior Executive with RoyalDutchShell for 30+ years and has extensive Global Chief Executive and Board membership experience.

He is a leader who is externally focused with a track record of building successful relationships with large multinational corporations, capable of business turnaround success and management of large scale construction projects.

Bill has strong and innovative strategic skills which are supported by a rigorous systematic approach to business planning, objective setting and results achievement.

Bill’s leadership values are based on respect for people supported by excellent coaching skills and he has applied them in novel organisational design and major change management successes.

Examples include a UK Company faced with a role change, a major change process to reduce staff by about 200 (60 per cent) and the introduction of new business processes. This was achieved with no interruption to customer service and the company developed a major customer programme which contracted levels of service based on staff’s analysis and agreement.

The initiation of the concept of moving from a country based business to a European business which was established within six months which identified and initiated significant cost saving programmes.

Bill was leader of a Business Development group which achieved success in setting up new ventures as well as disposal of non core activities. He created a novel design for the organisation and development processes. He introduced clear values for the organisation which were discussed and adopted by staff.

Since deciding to retire from RoyalDutchShell in 2005 Bill has been involved in a number of activities. He was a member of the Concept Development team for the LIFT project of the London International Festival of Theatre which was launched successfully in London in 2008. Bill is a Principal Industrial Fellow of the IfM University of Cambridge and in this role has delivered a large number of Strategic and Technological based projects for large FTSE companies. He is a member of the Consulting Partnership which provides
Jim Dawson
Director
INEOS Capital

Jim Dawson has a degree in chemistry, followed by a doctorate, from Oxford University. He spent most of his career in the Royal Dutch/Shell Group, starting in research, and then moving to product development, strategic planning and commercial management in several countries. He eventually became a Director of Shell Chemicals and Chairman of several of its global businesses. He was also CEO of Shell Renewable Energy, focusing on solar photovoltaics, biomass and wind power.

Following retirement from Shell he has been working with INEOS for several years and is a Director of INEOS Capital.

Rafat Malik
Head of Business Development
Faculty of Natural Science
Imperial College London

Rafat Malik joined Imperial in April 2007 and is currently Head of Business Development for the Faculty of Natural Science.

Rafat is an aeronautical engineer by training and has chartered status with the UK engineering council. He holds a BEng in Aeronautical Engineering and a MSc in Politics and International Relations and is currently pursuing a part time Masters/PhD in Intelligence, Science and Security.

Rafat’s career began with his first appointment with Smith’s Aerospace in 1996 as a primary flight controls design Engineer, and was seconded from the MoD to the US DoD to help develop the Joint strike fighter programme. Rafat progressed onto running a design team focused on commercial air platforms which required both technical and commercial expertise before leaving to join The McNeal Schwendler Corporation in 2001 where he held responsibility for growing the indirect business channel for engineering consulting within Europe and starting business development activities in the Middle East and emerging markets. He left in 2004, having grown the European consulting business by 70 per cent and having set up the first engineering applications distribution channel in the Middle. Rafat moved to Paris to head up the commercial aerospace, defence and security business for Pertinence Inc. a French engineering consultancy business where he lead a team of 12 engineers/scientists with a target to develop business models with EADS, BAE Systems, Arriva, Cogema, QinetiQ and other global engineering firms.

David Morgan
Chairman of the Advisory Board
Conduit Ventures Ltd

David Morgan is chairman of the advisory board of Conduit Ventures which is a venture fund focussed on high-efficiency energy storage, management, generation and supply. He spent much of his career at Johnson Matthey including 10 years as an executive director.

During his time at JM he held a number of senior positions, primarily corporate development and M&A related, but he also chaired the R&D Steering Committee, which was responsible for technology strategy, and had board level responsibility for a number of businesses. He served on the UK Science Forum which advised the Government on enhancing innovation in UK industry.

He has a degree in Natural Sciences from Trinity College Cambridge and qualified as a chartered accountant with KPMG.

Dr Sarah Shepley
Director of Corporate Partnerships
Development and Corporate Affairs
Imperial College London

Sarah Shepley is a BSc (1983-86) and PhD (1986-89) alumnus of Imperial’s Department of Chemistry and an MBA graduate of the Open University.

After gaining her PhD in 1989, Sarah joined ICI as a Senior Research Scientist in the Petrochemicals Division on Teesside. During the next 18 years she worked for ICI and DuPont in a number of petrochemicals and materials businesses, holding senior management positions in production, R&D, intellectual asset management and technology licensing, and working in a wide range of locations throughout the EU, Turkey, the Middle East and the CIS.

In June 2007 Sarah joined the Imperial Energy and Environment Office as Business Development Manager for the AtlanTICC Alliance, a unique UK-US R&D collaboration in Renewable Energy Technology Development between Imperial, Georgia Tech and the Oak Ridge National Laboratory.

In May 2009 she was appointed Director of Business Development for Imperial, and later become Director of Corporate Partnerships, in which role she leads the team that helps identify and win major multi-disciplinary corporate research funding bids for the University.

Jonathan Tyler
Managing Director
DC Advisory Partners Ltd and Chair of the Department of Chemistry Advisory Board

Jonathan joined DC Advisory Partners Ltd in September 2009 and heads the firms chemical practise, dealing with both M&A and restructuring transactions.

He has around fifteen years of chemical industry related finance experience, including extensive tenure years as a ranked research analyst, primarily heading the teams at Goldman Sachs.
Jonathan joined the firm from Houlihan Lokey, where he worked on the restructurings of INEOS, LyondellBasell and Chemtura. He was also expert witness for Dow Chemical in the Rohm & Haas vs. Dow case.

Jonathan is a graduate of both Imperial and London Business School. He chairs the advisory board of Imperial’s Department of Chemistry, and is on the development council of the National Theatre.

Malcolm P Weir PhD
Founder and Chief Executive Officer
Heptares Therapeutics Ltd

Malcolm has a BSc and PhD in biochemistry and biophysics from Imperial. He was Head of the Biomolecular Structure Department and then the Molecular Sciences Division of GlaxoWellcome with responsibility for 300 people engaged in target validation and lead discovery. During this time he led the application of structural biology and modelling to drug discovery, resulting in the advancement of clinical candidates to a wide range of diseases. He joined the structural bioinformatics and drug discovery company Inpharmatica Ltd as CEO in 2000, growing it from the spin-out stage to a 100-person company. Inpharmatica was sold to Galapagos NV in 2006. Malcolm was elected Visiting Professor of Biochemistry at Imperial in 1997, and to the Council of the UK Biotechnology and Biological Sciences Research Council in 2004.

John Wilkinson
Partner
ReedSmith

John is a member of the Life Sciences Health Industry Group, practising in the area of transactions. John’s practice focuses primarily on the life sciences sector advising pharmaceutical, biotechnology and medical technology companies on a wide range of IP, regulatory and transactional matters. Amongst other things, John’s practice has involved a number of highly complex alliances and joint ventures, co-promotional and co-marketing arrangements, distribution and supply agreements, together with the operational, IP and regulatory issues relating to such transactions.

John’s practice has involved advising pharmaceutical and biotechnology companies in the USA, UK, Denmark, Hungary, Switzerland, Portugal, New Zealand, Germany and Belgium.
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