The University of Nottingham

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School of Chemistry Annual Report 2011

www.nottingham.ac.uk/chemistry

Welcome

Welcome to the School of Chemistry at The University of Nottingham. We hope that you will enjoy reading about some of the School's many ongoing activities in our 2011 Annual Report.

The School of Chemistry at Nottingham is one of the leading departments in the UK and recognised internationally for its world-leading research portfolio, excellence in teaching and extensive engagement with Industry. This success is reflected in awards and prizes from professional bodies and international organisations. Underpinned by a strong foundation within the core Chemistry discipline and a highly collaborative interdisciplinary environment, the School has unique research and teaching strengths in:

- Healthcare and Drug Discovery,
- Green Chemistry and Sustainability,
- Low-Carbon Energy and Nanoscience, and
- Instrument Development and Analytical Science

The School of Chemistry has a thriving research environment with 160 postgraduate students and 60 post-doctoral fellows from all corners of the globe. These co-workers reflect the research activity of 38 academic staff supported by 30 technical staff. Chemistry is a truly multi-disciplinary science with researchers at Nottingham engaged in, and leading, major University-wide research initiatives with colleagues in the medical and biological sciences, in chemical engineering and in the nanosciences, to mention only a few.

An exciting development is that GlaxoSmithKline (GSK) and the University are to collaborate in constructing an innovative carbon-neutral laboratory that will be a Centre of Excellence for Sustainable Chemistry. It will focus on research that is of particular relevance to the pharmaceutical industry and which complements established expertise at the University. GSK has a number of existing relationships with us including providing support through postgraduate chemistry studentships, delivering a unique medicinal chemistry module in drug discovery to third year undergraduate chemists and offering opportunities for fourth year MSci project students to participate in live GSK research programmes. The University continues to provide GSK with high quality chemists for industrial placements, graduate and postgraduate roles.

"Nottingham is one of the best Universities in Britain, in fact the world, from a chemistry point of view"

Sir Andrew Witty CEO, GSK

Reflecting the cross-disciplinary nature of the School's research activities, chemistry researchers are also located in the £25 million SRIF-funded Centre for Biomolecular Sciences. To support its wide ranging research programmes, the School draws significant research funding from the chemical and pharmaceutical industries; the EU and the UK research councils (EPSRC and BBSRC); the Royal Society and other charities (Leverhulme Trust and Wellcome Trust) with research grants for each of the previous two years exceeding £10 million.

Professor Mark Searle
Head of School of Chemistry

Highlights

Dr Steve Liddle received the Sir Edward Frankland Fellowship (2011) from the RSC and the Bill Newton Award of the RSC Radiochemistry Group both for his contributions to the chemistry of f-block elements; he was elected Fellow of the Royal Society of Chemistry; he was elected Chairman of COST Action CM1006 and he received a Vice-Chancellor's achievement award. Read more of our achievements overleaf.

Honours and awards

The year 2011 has seen several significant individual awards and prizes including:

- Prof Sandy Blake was appointed Visiting Professor, RMIT University, Melbourne, Australia in December 2011
- Prof Neil Champness received a 2011-2016 Royal Society Wolfson Merit Award; he was listed in Times Higher 'Top 100' most cited Chemists in the last decade; and was appointed Visiting Professor at Institut Le Bel, University of Strasbourg, France, 2011
- Prof Mike George received the 2011 Craver Award of the Coblentz Society – an International Award in Vibrational Spectroscopy
- Prof Martyn Poliakoff CBE FRS was elected to the position of Foreign Secretary of the Royal Society and Vice-President of the Royal Society from 2011; RSC Nyholm Prize for Education 2011; he was elected Foreign Member of the Russian Academy of Sciences; he was awarded an Honorary DSc by Heriot Watt University and received a Vice-Chancellor's achievement award
- Prof Chris Moody held the 2011 Dr Paul Janssen Lectureship, Janssen Pharmaceuticals, Belgium and the Novartis International Lectureship
- Dr John Moses was appointed Distinguished Visiting Professor at King Saud University; he received the Thieme Chemistry Journals Award 2011 and was appointed "Honorary and Chair Professor of Natural Products and Biomimetic Chemistry", Institute of Biotechnology, Amity University, Noida, UP, India
- Prof Panos Soultanas was appointed visiting Professor in MIT, Boston
- Dr Sam Tang received the RSC's President's Award (2011) for outreach and public engagement in science; she received a Vice-Chancellor's achievement award and the Dearing Award
- Prof Simon Woodward chaired a Europe-wide COST Action covering 23 countries and over 400 scientists that has resulted in publication of a book covering many new concepts in Innovative catalysis

New research fellows

The School's success in attracting young scientists to Nottingham via competitive Fellowships has continued to inject vitality and dynamism into the teaching and research environment. Current early-career fellowship holders in the School include:

- Dr Elena Bichoutskaia (EPSRC Career Acceleration Fellow)
- Dr Libby Gibson (Royal Society Dorothy Hodgkin Fellow)
- Dr Andrei Khlobystov (Royal Society University Research Fellow, European Union Young Research Investigator and ERC Starting Grant Awardee)
- Dr Pete Licence (EPSRC Advanced Research Fellow)
- Dr Steve Liddle (Royal Society University Research Fellow and ERC Starting Grant Awardee) and Dr Rob Stockman (EPSRC Advanced Research Fellow)

2011 saw the addition of four new Research Fellows to the school staff:

Dr Sihai Yang joins the School as a Leverhulme Early Career Fellow, working on the development of porous traps for the capture of carbon dioxide and other gases

Dr David Robinson, also with a Leverhulme Early Career Fellowship, will be looking into better computational models and molecular probes for biological cell membranes

Dr Maria Gimenez Lopez, a Royal Society Dorothy Hodgkin Fellow, will be using her five-year fellowship to develop new nano-magnet-containing carbon structures for spintronics

Dr Andy Teale joins the School with a Royal Society University Research Fellowship, and will be investigating the development and implementation of extensions to density functional theory to tackle systems with several near-degenerate electronic configurations

Profiles of all our Research Fellows can be found on the Fellowships web pages: www.nottingham.ac.uk/chemistry/research/researchfellowships/fellows.aspx

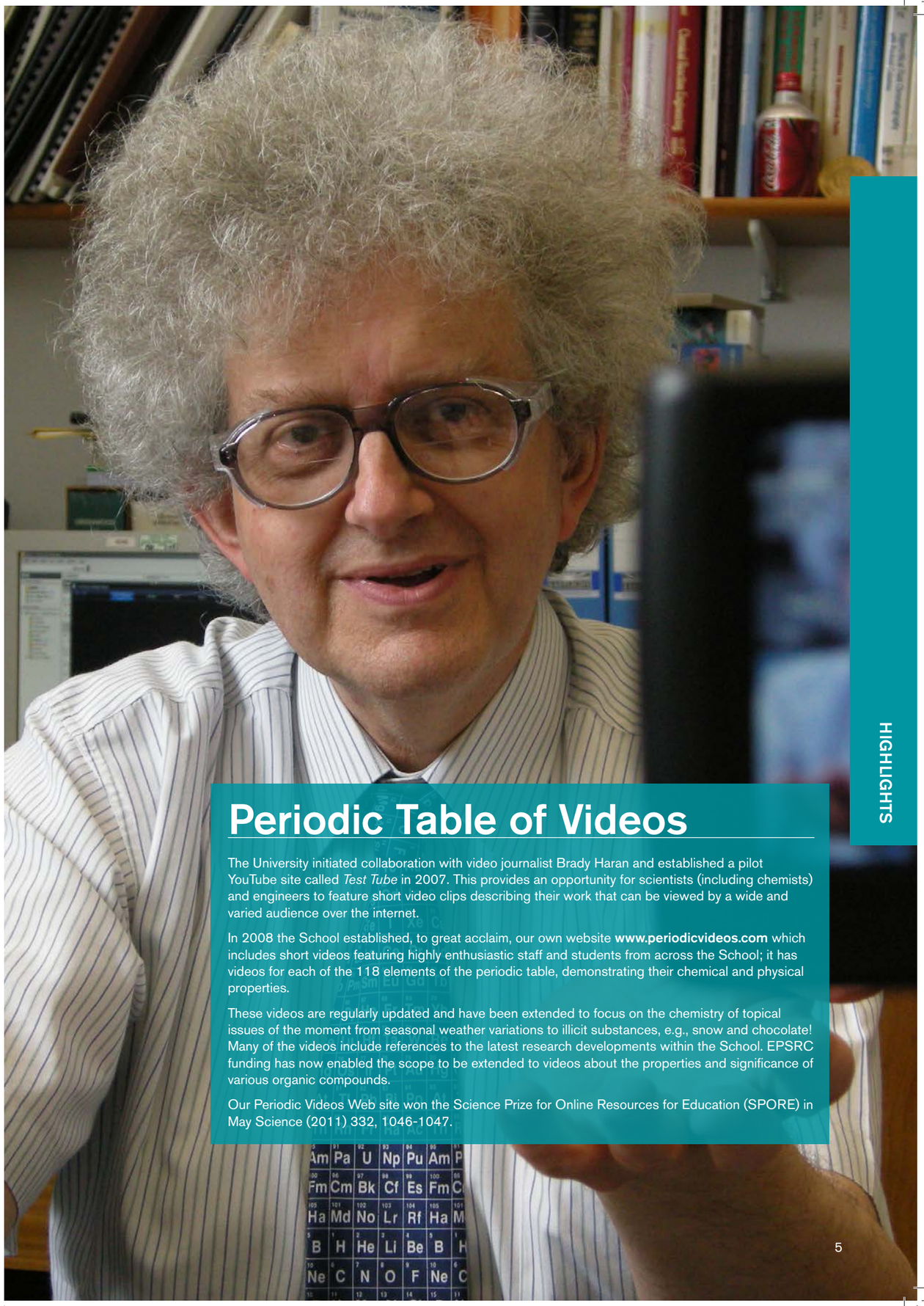
Infrastructure developments

GlaxoSmithKline (GSK) have given the University £12m towards the construction of an £18m innovative carbon-neutral laboratory for sustainable chemistry. The laboratory will be a Centre of Excellence for Sustainable Chemistry, based at Jubilee Campus, and will incorporate the latest technologies to allow it to be carbon-neutral over its lifetime. It will be built from natural materials and energy required to run the laboratory will be met by renewable sources such as solar power and use of sustainable biomass. Any excess energy created will provide enough carbon credits over 25 years to pay back the carbon used in its construction.

The research activity within the building will aim for the highest clean and green standards to minimise environmental impact and ensure that the chemistry is safe, energy efficient and, above all, sustainable. The building will also deliver teaching laboratories for advanced undergraduate projects and outreach to the wider community to embed sustainable chemistry principles in the next generation of scientists. The Centre of Excellence will serve as a global hub to catalyse new collaborations with other institutions and industry partners and will bring together leading UK academics, postgraduate and postdoctoral researchers and GSK chemists, developing expertise in sustainable chemistry. In addition, GSK will fund a new Chair in Sustainable Chemistry in order to further develop Nottingham's ambition to be the UK centre of excellence in this area. Construction of the laboratory will begin in the spring of 2013 and it is expected to be completed during 2014.

Recent investments in new instrumentation have seen a further upgrade of X-ray facilities to bring in a new powder diffractometer and single crystal diffractometers, including facilities for high pressure single crystal structural chemistry.

An investment of £1.8M has enabled existing 600 MHz NMR facilities located in the CBS building to be refurbished and to acquire both solid-state and rapid screening capabilities, as well as a new 800 MHz machine with cryoprobe facilities for structural biology. The latter is part of a University-wide Centre for High Resolution NMR spectroscopy, led by the School, which opened in the autumn of 2011.



Periodic Table of Videos

The University initiated collaboration with video journalist Brady Haran and established a pilot YouTube site called *Test Tube* in 2007. This provides an opportunity for scientists (including chemists) and engineers to feature short video clips describing their work that can be viewed by a wide and varied audience over the internet.

In 2008 the School established, to great acclaim, our own website **www.periodicvideos.com** which includes short videos featuring highly enthusiastic staff and students from across the School; it has videos for each of the 118 elements of the periodic table, demonstrating their chemical and physical properties.

These videos are regularly updated and have been extended to focus on the chemistry of topical issues of the moment from seasonal weather variations to illicit substances, e.g., snow and chocolate! Many of the videos include references to the latest research developments within the School. EPSRC funding has now enabled the scope to be extended to videos about the properties and significance of various organic compounds.

Our Periodic Videos Web site won the Science Prize for Online Resources for Education (SPORE) in May Science (2011) 332, 1046-1047.

Support for SMEs – The Chemistry Innovation Laboratory

The School has also been successful in securing £700k of ERDF funding to establish a "Chemistry Innovation Laboratory" which is focussing upon growing the School's interaction with regional Chemistry using SMEs.

The project is being managed by Dr. Freya Hine and facilitates access to a range of expertise and facilities within the School, aiming to support SMEs by helping them to innovate and grow. So far more than 70 companies have interacted with the project.

Public engagement

The School has a full-time Public Awareness Scientist, Dr Sam Tang, whose sole role is to communicate, excite and enthuse children of all age groups with the societal benefits and impact of science.

Dr Tang co-ordinates the School's extensive programme of public and schools outreach events in which staff volunteers also actively participate. These include staff and researcher visits to local schools. However, the majority of the activities are centred on the facilities within the School (for example, Salter' Science Fair, A-level Science Days, and many others). Dr. Tang is rapidly developing an international profile. She has been invited to lecture in Japan, Canada, Singapore, Dublin and, most recently, to 50 Norwegian science communicators at their annual conference in Cambridge organized by the Norwegian Research Council.

Heidi Dobbs has recently been appointed as the Royal Society of Chemistry's regional co-ordinator for the Midlands. Based within the Nottingham School of Chemistry, she supports the society's activities in the region, raising the profile of the wide range of educational resources the society offers. Heidi is a science champion, who works to promote the value of studying chemistry and open people's eyes to the impact it has on the world around us.

Commercialisation and business engagment

The School has strong and extensive links with a broad range of chemistry using industries. These include the fine chemical, pharmaceutical, medicinal, material and petrochemical industries but also food, health and personal care. These companies range from major multinationals (including GSK, Pfizer, AstraZeneca, Invista, General Motors, Unilever, Croda, Lucite, SI-Group, Shassun Pharma) to SMEs (Molecular Profiles, Lacerta Technology, Promethean Particles and Xenogesis).

Our interaction spans research, access to the School's services and facilities, feasibility studies, consultancy and in particular a significant level of industrial support for PhD studentships.

The School is a prolific provider of the next generation of skilled chemists for industry. For example, in the last 5 years, over 30 former PhD and postdoctoral scientists have been recruited to senior positions in the Pharmaceutical Industry. Approximately 40% of our PhD students are fully or partially supported through contributions from industry and benefit from placements in industry.

School of Chemistry Business Partnership Unit

The School has a unique, embedded Business Partnership Unit (BPU) which provides a focus for building an entrepreneurial culture among staff and students and engaging with potential users of research. The unit is led by a full time industry experienced Business Development Manager, Dr Trevor Farren, who is assisted by a number of postdoctoral Business Science Fellows, an approach pioneered in the School.

The unit continually monitors the output of research projects to identify potential impact and undertakes a range of activities (in collaboration with the University's technology transfer office) to develop them, including:

- undertaking short term feasibility studies in collaboration with industry
- supporting existing and developing new relationships with external partners
- securing investment for and undertaking knowledge transfer projects leading to technology licenses and spin-out company formation

The unit also acts as a focal point for business related enquires matching industry needs with capabilities within the school and supports a portfolio of business related training/ mentoring.

Business and entrepreneurial skills

This year, we have been successful in securing £50K funding from the HE STEM programme through the RSC to develop undergraduate modules and associated teaching resources designed to improve the business skills and awareness of undergraduate chemists and chemical engineers.

This work is being supported by the one-year appointment of a dedicated teaching fellow and the teaching resources will be made widely available through the RSC website. The School has also established a medicinal chemistry module in collaboration with GSK.

Careers evening

The School of Chemistry's annual careers evening provides an opportunity for current students to learn about the career decision of the School's previous graduates.

Our speakers this year included Jenny Unsworth (Patent Agent at Hepworth Browne and former Business Science Fellow), William Turner (Graduate medical student at Nottingham), Craig Bailey (Team Leader at BP), Caroline Cane (Policy Advisor at the Department for Education) and Catherine Lawrence (Policy Officer at the British Veterinary Association).

Undergraduate Prize Winners

Syngenta Awards are made annually to students of academic excellence in Chemistry. The 2011 winners were: **Rowena Howie, William Tipping, Petra Lindovska, Louisa Hitchen, Hannah Prydderch** and **Jennifer Smythe.**

The ***Robert Ficken Award*** is awarded to encourage the study of Chemistry at Undergraduate level by the most able students. The award is given annually to the most academically outstanding UK applicants who are admitted to study Chemistry at the University of Nottingham. The 2011 recipients were: **Claire Sycamore (winner), Christopher Wiseall (winner), Edward Rayner (runner-up), Stefan Paul Jones (runner-up), Alice Henley (runner-up)** and **Emma Billinger (runner-up)**.

The ***Takeda Cambridge Award*** is for the best overall performances by students taking the Medicinal and Biological Chemistry degree courses in year one and two. The 2011 winners were: **Jonathan Hunter, Bridie Dutton** and **Emma Blackham.**

This year, two awards were presented to second year students for their exceptional performance in year one laboratories: **Emily Elsey** and **Daniel Flint**.

Kipping Scholarships are available annually to second, third or fourth year undergraduate students whose performance in Chemistry is judged to have been distinguished. The 2011 recipients were: **William Tuttle, Joanna Kosalka, Adam Tibbles, Chloe Warsop, James Adams, Joshua Britton, Hannah Unitt, Elena Uteva, Katherine Haywood, Rebecca Blundell, Robert Straker** and **Peter Cleaves.**

Research

In the Research Assessment Exercise 2008, the School of Chemistry in Nottingham was ranked second in the UK for research quality (one below Cambridge and one above Oxford). Three quarters of the research outputs submitted were rated either as internationally excellent or world-leading.

Notable strengths included: 'the development of novel theoretical treatments of excited states of solvated molecules', 'the development of new synthetic methodology', and 'total synthesis'. The programme of interdisciplinary science at the interfaces of biology, nanoscience and chemical engineering were particularly commended.

Our research themes reflect strong collaborations and synergies between different researchers from across the School, and with other disciplines, demonstrated by jointly held research grants and co-authored publications.

These interactions strengthen both the core discipline and interdisciplinary science at a number of different interfaces. In many cases, they represent new and exciting emerging areas, or established internationally-recognised strategic activity, involving international leaders in their field at one end of the spectrum, and early career researchers (many holding competitive RCUK Fellowships) at the other end. Much of the activity sits within the EPSRC remit and interfaces with EPSRC Grand Challenge theme areas of 'sustainability', 'clean energy', 'carbon-capture', 'chemistry for life' and 'molecular systems engineering'. However, a substantial amount of activity is funded through the BBSRC and other sources. Key research themes across the School include:

Healthcare and drug discovery

Synthetic Methodology and Catalysis (new synthetic methodologies and routes to novel active molecules and complexes)

- Natural Product Synthesis
- Chemical and Structural Biology
- Medicines from Nature and drug discovery
- Polymers for drug delivery and biomedical applications

Green chemistry and sustainability

- Green Chemistry and Clean Technology
- Chemistry, catalysis and polymer synthesis in supercritical fluids and ionic liquids
- Impregnation of polymers with other species using supercritical fluids
- Sustainable chemical processes and processing (including catalysis, microwave synthesis, renewable feedstocks)

Low-carbon energy and nanoscience

- Co-ordination Chemistry and Catalysis
- Chemical NanoSciences single molecule imaging, assembly in the solid state and on surfaces
- Nanostructured and nanoporous materials for hydrogen storage, production and energy applications
- Photochemistry, photophysics and electron transfer for water splitting and carbon capture
- Carbon nanostructures and dye sensitised solar cells
- f-block element chemistry

Instrument development and analytical science

- Theoretical and Computational Chemistry
- Development of spectroscopic methods to probe excited states and reaction mechanisms
- Physical Chemistry and Materials Science
- Fundamental gas phase studies on molecular dynamics, interactions and reactive intermediates
- Electrochemistry
- Astrophysical Chemistry

This activity is reflected in over 800 journal publications since January 2008 attracting >3400 citations at 4.2 citation per paper. Over a third of our staff are highly cited chemists (with >800 citations on papers published in the last 10 years).

RESEARCH

Dr Nicholas A Besley

Theoretical chemistry; quantum chemistry; density functional theory; ab initio molecular dynamics; spectroscopy

The central theme of our research is the development of quantum chemical methods to study a wide range of problems ranging from accurate calculations of the spectroscopy of small molecules to understanding the function of metalloproteins. The group exploits High Performance Computing, which has made quantum chemical calculations tractable for large systems, providing an opportunity to contribute to many areas of chemistry. We work closely with the commercial software package Q-CHEM, and the developments that the group make are implemented within this package. Key active areas of research are:

- modelling electron transfer in blue copper proteins
- development of new exchange-correlation functionals with density functional theory for the calculation of x-ray absorption and x-ray emission spectroscopy and their application to large systems
- new methods for the study of molecular dynamics in electronically excited states
- new approaches to treat anharmonic molecular vibrations within extended systems.
- treatment of dispersion interactions within density functional theory

The group is also actively involved in applying quantum chemistry as part of collaborative projects with colleagues in the School of Chemistry. These include the study of graphene and nanotubes (with Drs Kholobystov and Bichoutskaia), the modelling of fluorescent molecules within phospholipid membrane bilayers (with Prof Hirst, Dr Robinson and Prof O'Shea (School of Biology)) and the study of the infrared spectroscopy of molecules in electronically excited states (with Prof George).

Highlight publications

Robinson, D. and Besley, N. A. (2011) Theoretical simulation of the spectroscopy and dynamics of a red copper protein. Faraday Discussions. 148, 55-70

Chamberlain, T. W., Meyer, J. C., Biskupek, J., Leschner, J., Santana, A., Besley, N. A., Bichoutskaia, E., Kaiser, U. and Khlobystov, A. N. (2011) Reactions of the inner surface of carbon nanotubes and nanoprotrusion processes imaged at the atomic scale. Nature Chem. 3, 732-737

Dr Elena Bichoutskaia

Theoretical prediction of materials properties; computational modelling of carbon nanomaterials; electromechanical devices at the nanoscale; weak van der Waals forces; gas storage and interactions in porous solids

In 2010-2011, two new theoretical models have been developed in my group, which underpin fundamental interactions taking place at the nanometre scale. A general solution to the fundamental problem of the attraction between like-charged dielectric nanoparticles has been proposed. This is the first time a comprehensive solution to this problem has been presented, and it has the potential to transform our understanding of how charged nanoparticles interact in the gas phase and solutions.

Studies of nanoparticles have opened new avenues for exploration of the principles that underpin the transition from the gas phase to the solid state. The capability of nanoparticles to modify their shape in order to minimize the free energy leads to structure modifications that can be observed on a time scale accessible by electron microscopy techniques. A novel computational methodology has been developed in my group, which has an advantage over the state-of-the-art image simulation techniques in its ability to simulate the dynamics of structural transformations under the influence of the electron beam.

The proposed theoretical frameworks offer solutions to problems across wide-ranging disciplines. The application areas include the electrostatic charging of pharmaceutical powders during manufacture and handling; the charge scavenging in the formation of solar systems; self-assembly of charged nanoparticles in solutions; proton transfer in biological molecules; structure-property correlations of nanomaterials; and design of innovative oxidation catalysts using inorganic polyoxometalates.

Highlight publications

Stace, A. J. and Bichoutskaia, E. (2011) Treating highly charged carbon and fullerene clusters as dielectric particles. Phys. Chem. Chem. Phys. 13, 18339-18346

Chuvilin, A., Bichoutskaia, E., Gimenez-Lopez, M. C., Chamberlain, T. W., Rance, G. A., Kuganathan, N., Biskupek, J., Kaiser, U. and Khlobystov, A. N.(2011) Self-assembly of a sulphur-terminated graphene nanoribbon within a single-walled carbon nanotube. Nature Materials. 10, 687-692

Prof AJ (Sandy) Blake

High pressure coordination chemistry theory; metal-organic frameworks; structural chemistry; synchrotron radiation

We are engaged in a systematic search to discover new phenomena, primarily by means of applying high pressures of up to 150,000 atmospheres to single crystals of transition metal coordination complexes. The phenomena we have observed so far include changes in geometry at metal centres, polymerisation, conformational rearrangements and colour changes which can be unexpected, extreme or multiple. We have also been able, using pressure alone, to induce close pi-pi interactions and strong pyramidalisation at the bridgehead carbon atom in a phenyl ring, which raises interesting questions about its hybridisation. We use high-level DFT calculations (with McMaster) to help us understand these processes. Current work also aims to explain the extreme sensitivity of certain encapsulated metal complexes to changes in their environment.

We are also interested (with Schröder and Champness) in the structural characterisation of metal-organic and related frameworks for applications in gas storage, including carbon capture and hydrogen containment for clean transport. This involves the use of both in-house instrumentation and central facilities (synchrotrons and neutron sources) in the UK and overseas. We are also combining our interests in high pressure science and metal-organic frameworks to investigate their behaviour towards absorbent molecules under pressure.

Highlight publications

Kathirgamanathan, P., Surendrakumar, S., Antipan-Lara, J.S. Ravichandran, S., Reddy, V.R., Ganeshamurugan, S., Kumaraverl, M., V. Arkley, V., Blake, A.J. and Bailey, D. (2011) Discovery of two new phases of zirconium tetrakis(8-hydroxyquinolinolate): synthesis, crystal structure and their electron transporting characteristics in organic light emitting diodes (OLEDs). J. Mater. Chem. 21, 1762–1771

Blake, A. J., McMaster, J., van Slageren, J., Moro, F., Mills, D. P., Lewis, W., and Liddle, S. T. (2011) A delocalised arene-bridged diuranium single molecule magnet. Nature Chem. 3, 454–460

Dr Jason E Camp

Sustainable synthetic chemistry; total synthesis; sugar derived metal nanoparticles; multifaceted catalysis

Dr. Camp's current research is focused on the development of efficient methods for selective bond formation that minimise time, expense and environmental impact. Our research programme can be subdivided into two main areas: (a) development of highly active, renewable metal nanoparticle catalysts derived from simple sugars and (b) a multifaceted catalysis approach to synthesis that optimises synthetic efficiency.

Our studies on sugar derived catalytic nanoparticles, which are done in collaboration with Walsh, Thielemans, Khlobystov and Parmenter, are focused on harnessing the reducing potential of renewable sugars to power synthetic transformations. The reduction potential of renewable sugars is being harnessed to form catalytically active metal (0) nanoparticles (M^0NPs) from metal precatalysts and turn over the catalytic cycle to regenerate the active catalyst under aqueous conditions. Harnessing the multiple reducing equivalents of reducing sugars to drive chemical transformations results in: (a) existing catalytic processes being made more cost efficient in terms of time, expense and waste (b) the development of novel, high impact catalytic processes.

We are also actively investigating mild, sustainable and environmentally benign processes that utilise noble metals for catalysis. Specifically, systems in which one catalyst can activate more than one mechanistically distinct step in a reaction process, multifaceted catalysis (MFC) are being developed. A MFC approach allows for the conversion of simple starting materials to added-value compounds, whilst limiting the overall costs in terms of time, expense and waste. A recent example from our group is the gold-MFC process for the construction of pyrroles, which involves activation of an alkyne towards nucleophilic addition of an oxime and subsequent catalysis of the conversion of the newly formed *O*-vinyl oxime to the pyrrole. It was shown that the same gold catalyst activates both of these processes. In comparison to existing protocols the gold-MFC process gave higher yields, increased substrate scope and proceeded at significantly lower temperatures.

Highlight publications

Ngwerume, S., and Camp, J. E. (2011) Gold-Catalysed Rearrangements of *O*-Vinyl Oximes for the Synthesis of Highly Substituted Pyrroles. Chem. Comm. 47, 1857–1859

Chung, W., Lindovská, P., and Camp, J. E. (2011) A one-pot synthesis of α-formyl-α-allylacetates via nucleophilic catalysis. Tetrahedron Lett. 52, 6785–6787

Prof Neil R Champness

Supramolecular chemistry; crystal engineering; guest molecular entrapment; nanostructure fabrication

Research in the Champness group concerns all aspects of molecular organization, with particular emphasis on surface supramolecular assembly and control of solid state structure via crystal engineering. Particular targets of our work are guest molecular entrapment, whether in the solid-state or on surfaces, and nanostructure fabrication for applications in hydrogen storage and information storage exploiting molecular self-assembly.

Our studies of surface-based self-assembly processes, in collaboration with Beton (Nottingham, Physics), using supramolecular interactions pursue the control of organization at the molecular level. Our focus develops the formation of nanostructured arrays that contain both chemical and physical information, exploiting information encoded within the molecular structure. Targets include the development of systems that allow specific entrapment of guest molecules that can act as information carriers and the expansion of our recent discovery of random tiling arrangements that provide a link between ordered structures and quasi-crystalline arrays.

Our studies of metal-organic frameworks (MOFs) have two key strands: the synthesis of MOFs that contain photoactive components, in collaboration with George, and gas storage systems, including hydrogen gas, in collaboration with Schröder. Building on our original demonstration of the modification of photoactivity as a result of the MOF environment, we are targeting the development of new photoactive MOFs which provide a platform for controlling photochemical, and photophysical processes allowing direct evaluation of unusual reaction processes and facilitating new pathways to charge separated states.

Highlight publications

Blunt, M. O., Russell, J. C., Gimenez-Lopez, M. C., Taleb, N., Lin, X., Schröder, M., Champness, N. R., Beton, P.H. (2011) Guest-Induced Growth of a Surface-Based Supramolecular Bilayer. Nature Chem. 3, 74–78

Slater, B.J., Davies, E. S., Argent, S.P., Nowell, H., Lewis, W., Blake, A.J., Champness, N. R. (2011) A Perylene Diimide Rotaxane: Synthesis, Structure and Electrochemically-Driven De-threading. Chem. Eur. J., 17, 14746-14751

Dr Ross M Denton

Catalysis; organic synthetic methods; organophosphorus catalysis; organophosphorus chemistry; natural product synthesis

The main activities of my research group are developing new reactions (particularly new catalytic reactions), the study of organophosphorus compounds using computational chemistry (particularly phosphoranes) and the total synthesis of natural products that show neuroregenerative properties.

New catalytic reactions and organophosphorus chemistry. In three recent publications we demonstrated the first examples of catalytic phosphorus-based hydroxyl activation and nucleophilic substitution in the form of the first catalytic Appel reaction. This has demonstrated that catalysis of phosphorus-mediated reactions – in which the very strong P=O bond must be cleaved – is possible at room temperature with catalyst loadings as low as 1 mol%. This has overturned the belief that catalysis of phosphorus-based reactions would not be possible under synthetically relevant conditions. Furthermore, it has transformed phosphine oxides (the stoichiometric by-products in classical phosphorus-mediated reactions) from waste products into catalysts and constitutes part of a newly emerging area of catalysis.

Total synthesis of natural products. The first synthesis of dunnianol, OMe-honokiol and the shortest and most efficient synthesis of honokiol have also recently been achieved. We are examining their role in neuroregeneration in collaboration with The Cambridge Centre for Brain Repair.

Highlight publications

Denton, R. M., Jie, A., Adeniran, B., Blake, A. J., Lewis, W. and Poulton, A. (2011) Catalytic Phosphorus(V)-Mediated Nucleophilic Substitution Reactions: Development of a Catalytic Appel Reaction. J. Org. Chem. 76, 6749-6767

Denton, R. M., Scragg, J. T., and Saska, J. (2011) A Concise Synthesis of O-methyl Honokiol. Tetrahedron Lett. 52, 2554-2556

Dr James Dowden

Chemical biology, inhibitor design, natural product synthesis, synthetic methodology

We are prospecting for small molecules that may be of utility for chemical dissection of biological processes in living cells and organisms, or ultimately as new medicines. This approach involves two complementary activities: i) rational design of small molecule modulators of enzymes based on their co-substrates; ii) design of original synthetic methods that offer expedient access to new drug-like molecular scaffolds inspired by natural products.

i) Inhibitor Design: Protein arginine methyltransferases PRMTs are of significant contemporary interest, especially in light of their role in epigenetic regulation of cell status. Silencing of specific PRMT genes has been shown to reduce growth of bladder and lung cancer cells. We have developed small molecules that occupy binding sites for AdoMet co-factor and arginine protein substrate. Biological evaluation by collaborators confirmed that the compounds are selective and potent PRMT inhibitors.

We performed virtual docking experiments that suggest the binding mode of these compounds. Overlay of structures of two different PRMTs revealed a single amino acid difference close to the binding channel that may explain why these relatively simple prototype compounds are selective. We are currently seeking more detailed binding studies using techniques such as isothermal titration calorimetry, NMR, X-ray crystallography etc. We are busy improving the properties of the inhibitors, for example to make them cell permeant. We are keen to develop collaborations with biologists with interests in methyltransferases.

ii) New synthetic methods: Medicinal alkaloids are a potentially rich source of inspiration for such scaffolds. We are currently investigating new reactions of pyridinium salts that provide rapid access to alkaloids including: a) novel cycloaddition reactions between pyridinium ylides and various dipolarophiles, leading to complex indolizidine structures; b) a novel conjugate addition, ring closing sequential reaction of pyridinium salts, leading to quinolizidine alkaloids.

Highlight publications

Dowden, J., Pike, R. A., Parry, R.V., Hong, W., Muhsen, U. A., and Ward S. G. (2011) Small Molecule Inhibitors That Discriminate Between Protein Arginine N-Methyltransferases PRMT1 and CARM1. Org. Biomol. Chem. 9, 7814-7821

Hong, W., and Dowden, J. (2011) Facile synthesis of N-6 adenosine modified analogue toward S-adenosyl methionine derived probe for protein arginine methyltransferases. Chin. Chem. Lett. 22, 1439-1442

Prof Mike W George

Spectroscopy, Organometallic and Coordination Chemistry; Photochemistry, Process and Reaction Monitoring; Analytical Chemistry

Our group works at the interface between Inorganic, Physical and Analytical Chemistry and a large part of activity focuses on exploiting photochemistry and spectroscopy, particularly time-resolved spectroscopy, to characterise intermediates and elucidate reaction mechanisms processes with particular emphasis on organometallic and coordination chemistry. Current research projects fall into different areas including the activation of small molecules (particular alkanes and CO_2) and probing reaction mechanisms including excited states and electron and energy transfer particularly for solar energy applications. We have projects using vibrational spectroscopy for the elucidation of electron/energy transfer in DNA. We are also exploiting the unique properties of supercritical fluids, in collaboration with colleagues in Southampton, for the electrodeposition of metals and semiconductors from supercritical fluids for nanomaterial deposition.

Scientific highlights in 2011 include major advances in the area the formation of organometallic alkane complexes and the mechanism alkane activation. Collaboration with colleagues at York allowed the characterisation of the first organometallic first row alkane complex by IR and NMR spectroscopy and a detailed study on the mechanism of C-H activation of alkanes using $Cp'Rh(CO)_2$ (Cp' = Cp or Cp*) shed new insight into this important reaction. A range of studies have been reported where we have used a combination of photochemistry and fast IR spectroscopy to elucidate important aspects of the structure of excited states and the reactivity of organometallic intermediates. Other outputs include the ultilisation of IR spectroscopy to interrogate electron transfer reactions in DNA; the development of a new IR approach to measuring phase behaviour of high pressure fluids where a single sensor can detect two different transitions. A key aspect for part of our studies is the use of solar energy and research in the area of solar fuels including the development of new catalytic systems for photochemical CO_2 reduction; development of continuous flow reactions for photochemical oxidation reactions and an investigation into the feasibility of using CO_2 from Carbon Capture and Storage to reduce the energy costs of performing reactions in supercritical fluids on an industrial scale.

Highlight publications

Calladine, J. A., Duckett, S. B., George, M. W., Matthews, S. L., Perutz, R. N., Torres, O., and Khuong, K. Q. (2011) Manganese Alkane Complexes: An IR and NMR Spectroscopic Investigation. J. Am. Chem. Soc. 133, 2303-2310

Batool, M., Martin, T. A., Abu Naser, M., George, M. W., Macgregor, S. A., Mahon, M. F., and Whittlesey, M. K. (2011) Comparison of the Photochemistry of Organometallic N-heterocyclic Carbene and Phosphine Complexes of Manganese. Chem. Commun. 11225-11227

Dr Elizabeth A Gibson

Dye-sensitized solar cells; molecular devices; molecular synthesis; nanostructured NiO; photochemistry; electrochemistry

Research in the Gibson group aims to significantly improve the conversion efficiency of dye-sensitized solar cells, by developing tandem devices with two photoelectrodes, one harvesting the high energy photons, and the other harvesting the low energy photons. This allows us to increase the photovoltage, whilst maximizing light harvesting across the solar spectrum. The current on both sides must be matched and so the photocurrent from the p-type electrode must be increased to that of typical n-type DSCs. However, the performances of p-type DSCs are significantly lower than the n-type TiO_2 analogues. The main limitations have been the small potential difference between the valence band of the NiO, p-type semiconductor, and the redox potential of the electrolyte and the faster charge-recombination reactions compared to the TiO_2 system. We are addressing these limitations, by improving the quality of the NiO electrodes, substituting the triiodide/iodide electrolyte for more suitable alternatives and engineering new dyes specifically for the p-type system. In addition we perform fundamental studies on the mechanism of the photo-electrochemical reactions involved using transient spectroscopy and electrochemistry.

In the last 12 months we have established a laboratory for the construction and characterisation of the solar cell devices and welcomed the first two members of my group, Dr Jean-François Lefebvre and Christopher Wood. Both are currently synthesising new dyes specifically for photocathode sensitization. We have also developed some new NiO nanostructures which we hope will increase the cell performance. In 2011 we have significantly increased our understanding of the implications of different electrolytes on the device efficiency leading to the publication of three research articles and the recent submission of three further manuscripts. We are using this mechanistic insight to better engineer our sensitizers to optimise the photoconversion efficiency.

Highlight publications

Boschloo, G., Gibson, E. A., and Hagfeldt, A. (2011) Photomodulated Voltammetry of Iodide / Triiodide Redox Electrolytes and its Relevance to Dye-sensitized Solar Cells. J. Phys. Chem. Lett. 2, 3016–302

Gibson, E. A., Smeigh, A. L., Le Pleux, L., Hammarström, L., Odobel, F., Boschloo, G., and Hagfeldt, A. (2011) Cobalt polypyridyl-based electrolytes for p-type DSCs. J. Phys. Chem. C. 115, 9772-9779

Dr Maria del Carmen Gimenez-Lopez

Spintronics; molecular magnetism; carbon nanostructures; nanoparticles

Since 1 October 2011, I started a new project titled, *Nano-Magnets in Carbon Nanostructures* as Royal society Dorothy Hodgkin Research Fellow. My current research is focused on a new area of technology called spintronics, which is a branch of electronics that is aimed at exploiting the property of the spin of the electron in addition to its charge. It is important because of their potential advantages, such as: i) the increased data processing speed, ii) the decreased electric power consumption and iii) the possibility to create computer memories that can retain the stored information, even when not powered. However, many practical aspects in this area are hindered because of the lack of suitable materials.

My fellowship is targeted at developing a totally new class of materials using two different components: i) Nanotubes made of carbon which can transport both properties of the electrons (charge and spin) over long distances. ii) Nano-sized magnets that can detect or create magnetic fields, and record and store information. One of the most exciting challenges of my project is to create nanoscale architectures using these tiny hollow wires (10,000 times thinner than a human hair) made of carbon. These will be “nano test tubes” to encapsulate and store nano-sized magnets. Very recently together with Dr. Khlobystov we have demonstrated the successful encapsulation of Mn_{12} single-molecule magnets in carbon nanotubes, yielding a new type of hybrid nanostructure that combines all the key single-molecule magnet properties of the guest molecules with the functional properties of the host nanotube.

Before October, I have been working as Marie Curie Fellow in the Carbon Nanomaterials group of Dr. Khlobystov. In this project, I studied the interactions between molecules or nanoparticles and nanotubes and successfully developed a general methodology for confinement of complex molecular structures within nanotubes, forming unique novel types of hybrid nanomaterials with the potential for electronic applications.

Highlight publications

Gimenez-Lopez, M. C., Chuvilin, A., Kaiser, U., and Khlobystov, A. N. (2011) Functionalised endohedral fullerenes in carbon nanotubes, Chem. Commun. 47, 2116-2118

Gimenez-Lopez, M. C., Moro, F., La Torre, A., Gomez-Garcia, C. J., Brown, P. D., van Slageren, J., and Khlobystov, A. N. (2011) Encapsulation of single-molecule magnets in carbon nanotubes. Nature Commun. 2, 407

Prof Christopher J Hayes

Organic chemistry; natural product synthesis; continuous flow chemistry; carbenes; modified nucleic acids; drug discovery

We have core expertise in the chemical synthesis of biologically important target molecules, and work extensively in the area of natural product chemistry. The successful enantioselective syntheses of TAN1251A, (+)-lactacystin, (-)-cephalotaxine, procyanidin B3, (+)-cymbodiacetal and the core structures of FR901483 and dihypoestoxide are significant recent achievements. In an on-going collaboration with Dr Fray (Plant Sciences) we are studying the production, and chemical modification of members of the taxane family of diterpenoid natural products in genetically modified plants (i.e. tomato). In addition to our natural product work, we also develop new reaction methodology exploiting the chemistry of reactive intermediates (i.e. carbenes and nitrenes) and we are using continuous flow chemistry to enable these intermediates to be used in a safe and convenient manner.

In addition to building core strength in natural product chemistry, we have developed a diverse portfolio of research at the chemistry/biology interface, with particular emphasis on nucleic acid chemistry and biology. Our ability to synthesise bespoke modified oligonucleic acids on large scale has led to a productive research collaboration with Prof Brook (Genetics) focussing upon the use of oligonuleic acids for the treatment of myotonic dystrophy, which is the most common form of muscular dystrophy in adults. Furthermore we have also developed new synthetic methodology for the synthesis of methylated RNA sequences that have significance in the rapidly emerging area of epigenetics.

Highlight publications

Kruse, S., Zhong, S., Bodi, Z., Button, J., Alcocer, M. J. C., Hayes, C. J., Fray R. (2011) A novel synthesis and detection method for cap-associated adenosine modifications in mouse mRNA. Scientific Reports. 1,126

Bartrum, H. E., Blakemore, D. C., Moody, C. J., Hayes, C. J. (2011) Rapid Access to a-Alkoxy and a-Amino Acid Derivatives via Safe Continuous-flow Generation of Diazoesters. Chem. Eur. J. 17, 9586-9589

Prof Jonathan D Hirst

Computational chemistry; quantum chemistry; molecular simulation; computer-aided molecular design; protein spectroscopy

Our research focuses on the application of computational chemistry to challenging problems in biology. This field is one of the most vibrant in computational biology, fuelled by the dramatic progress in computer hardware development and the deluge of biological data emerging from genome sequencing. Our research spans a wide range, from the quantum chemistry of small molecules and the spectroscopic properties of proteins, to the application of state-of-the-art statistical and computer science methodology to problems in drug design and bioinformatics. Much of the research centres on understanding how proteins fold into their preferred biologically active shapes. The protein folding problem has been called “the second half of the genetic code” and, if solved, it would revolutionise molecular biology and medicine by permitting real exploitation of genome sequence data.

In 2011, we have been involved in many collaborative projects. Molecular dynamics (MD) simulations have been used to study the folding of a small protein (in collaboration with Prof Searle, Chemistry) and the binding of di- and tri-peptides to a protein dimerisation interface (with Prof Shaw, Biomedical Sciences). The role of water in such simulations has been investigated (with Prof Garrahan, Physics) and so-called ab initio MD simulations have allowed us to predict the spectroscopy of small peptides (with Dr Besley, Chemistry, and Prof Gaigeot, Université d’Evry). MD simulations have also been used to study phospholipid bilayers (with Dr Robinson and Dr Besley, Chemistry, and Prof O’Shea, Biology). Monte Carlo, a different simulation technique, has been applied to study mixtures of small molecules, including

Highlight publications

Chen, P., Evans, C.-L., Hirst, J. D. and Searle, M. S. (2011) Structural insights into the two sequential folding transition states of the PB1 domain of NBR1 from phi-value analysis and biased molecular dynamics simulations. Biochemistry. 50, 125-135

Gaigeot, M.-P., Besley, N. A. and Hirst, J. D. (2011) Modelling the infrared and circular dichroism spectroscopy of linear and cyclic diamides. J. Phys. Chem. B. 115, 5526–5535

Prof Steven M Howdle

Polymer Synthesis; Polymer Processing; Drug Delivery; Tissue Engineering; Supercritical Fluids

Our group is focussed on the applications of supercritical carbon dioxide ($scCO_2$) to polymer synthesis and polymer processing. We have developed a wide range of high pressure equipment, from micro-litre to litre scale, and we have developed new techniques to allow us to exploit the unique properties of $scCO_2$ for a wide range of potential applications.

This year we have discovered a range of hydrocarbon polymers that show very good solubility in $scCO_2$. These are important because up till now only fluorocarbon and silicone based polymers have shown appreciable solubility and this has been a hurdle from both a cost and environmental aspect to the further development of $scCO_2$ processing on the industrial scale.

We have also continued to develop scaffolds for tissue engineering applications and have demonstrated that highly potent and thermally labile growth hormone can be encapsulated successfully using $scCO_2$ to create polymeric drug delivery devices. This work is being commercialised, see www.criticalpharmaceuticals.com.

Highlight publications

Popov, V. K., Bagratashvili, V., N., Krotova, L. I., Rybaltovskii, A. O., Smith, D. C., Timashev, P. S., Yang, J., Zavorotnii, Y. S., and Howdle, S. M. (2011) A Route to Diffusion Embedding of CdSe/CdS Quantum Dots in Fluoropolymer Microparticles. Green Chemistry. 13, 2696-2700

Birkin, N. A., Arrowsmith, N. J., Park, E. J., Richez, A. P., Howdle, S. M. (2011) Synthesis and Application of New CO2-Soluble Vinyl Pivalate Hydrocarbon Stabilisers via RAFT Polymerisation. Polymer Chemistry 2, 1293 - 1299

Dr Derek J Irvine

Polymerisation, Catalysis, Interfacial Chemistry, Microwave-assisted chemistry, Process scale-up

Derek Irvine's work focuses primarily in the areas of novel polymer synthesis, catalysis and processing, where the latter area specifically concerns overcoming the problems in scaling up of Controlled Radical Polymerisation. This involves the synthesis and manufacture of Hyperbranched polymers, design and use of non-migratory surfactant systems for composite manufacture and also the effects upon polymerization of conducting them in alternative solvent systems such as Ionic Liquids, dense phase fluids and Fluorous Phases. He is now part of the NCIMP (National Centre for Industrial Microwave Processing) in which he leads the research programmes dedicated to microwave promoted polymerisation. This latter area is focused on improving the sustainability of chemistry by identifying novel low energy and continuous manufacturing processes.

Highlight publications

Kamaruddin, M. J., El harfi, J., Dimitrakis, G., Nguyen, N. T., Kingman, S. W., Lester, E., Robinson, J. P. and Irvine, D. J. (2011) Continuous direct on-line reaction monitoring of a controlled polymerisation via dielectric measurement. Green Chemistry, 13, 1147-1151

Parrott, A. J., Bourne, R. A., Akien, G. R., Irvine, D. J., and Poliakoff, M. (2011) Self-Optimizing Continuous Reactions in Supercritical Carbon Dioxide. Angew. Chem. Intl Ed. 50, 3788-3792

Prof Robert G Jones

Surface science; ionic liquids; liquid surfaces; surface structure;synchrotron radiation; X-ray standing wave

Liquid surface science uses ultra-high vacuum surface science methods to study liquid surfaces at the molecular level. This area of research, which only started about seven years ago, uses ionic liquids (ILs) as they do not evaporate under ultra-high vacuum and are electrically conducting (allowing charged particle techniques to be applied to them). The past few years have involved exploratory studies of ILs, leading to seminal works on their evaporation (energetics and the nature of the gas phase itself) and surface characterization, chemistry and structure (by line of sight mass spectrometry, ultra-violet and X-ray photoelectron spectroscopies, etc.).

At present we are studying the adsorption and absorption of gases onto and into ionic liquids that are directly relevant to their use as carbon capture agents, capture agents for other gases (e.g. SO_2), gas separation media and in SILP. We are also embarking on a study of ultra-thin IL layers on solid surfaces, which are directly relevant to the realization of two-dimensional solvents and the uses they would have in lubrication, nanoscience and nanotechnology. We collaborate closely with Dr. Licence and Prof. Moriarty (Physics).

Highlight publications

A. W. Taylor, K. R. J. Lovelock, R. G. Jones and P. Licence. (2011) Borane-substituted imidazole-2-ylidenes: synthesis in vacuo. Dalton Trans. 40, 1463-1470

Deyko, A., Lovelock, K. R. J., Licence, P. and Jones, R. G. (2011) The vapour of imidazolium–based ionic liquids: a mass spectrometry study. Phys. Chem. Chem. Phys. 13, 16841-16850

Dr Deborah L. Kays

Main group chemistry; transition metal chemistry; organometallics; low-coordinate; metal-metal bonding; reactivity

Research in the Kays group involves the stabilisation of low-coordinate and binuclear main group and transition metal species. These highly reactive compounds are of great importance not only from a fundamental structure/bonding viewpoint, but also because of their potential industrial applications e.g. in catalysis. Particular interest is in the development of new synthetic methodologies and the use of novel ligand systems to support unsaturated and/or highly reactive complexes. The analysis of these complexes through spectroscopic, structural and computational studies, and the investigation of their fundamental patterns of reactivity, will lead ultimately to the exploitation of these species in areas such as catalysis and materials chemistry.

Recent work within the Kays group has led to the stabilisation of rare examples of two- and three-coordinate transition metal aryl complexes such as $(2,6\text{-}Mes_2C_6H_3)_2M$ (M = Mn, Fe, Co; Mes = $2,4,6\text{-}Me_3C_6H_2$) and $(2,6\text{-}Naph_2C_6H_3)_2Co(OEt_2)$ (Naph = $1\text{-}C_{10}H_7$). Investigation of the reactivity of these m-terphenyl complexes is allowing us to access to novel Zintl ions and organic molecules such as sterically encumbered benzophenones via M–C bond breaking and insertion reactions. Our main group investigations follow two main strands: the stabilisation of highly reactive complexes of the alkaline earth elements – in particular Grignard analogues as precursors to new Group 2 metal-metal bonds and the synthesis of new borylene ligands, featuring boron in the +1 oxidation state, and their transition metal complexes.

The reaction of the three-coordinate cobalt(II) terphenyl complex with CO provides a new and clean route to highly encumbered benzophenones.

Highlight publications

Blake, A. J., Lewis, W., McMaster, J., Moorhouse, R. S., Moxey G.J., and Kays, D. L. (2011) Amido Analogues of Zincocenes and Cadmocenes. Dalton Trans. 40, 1641-1645

Kays, D. L. (2011) Recent Developments in Transition Metal Diaryl Chemistry. Dalton Trans. 40, 769-778

Prof Andrei N. Khlobystov

Carbon nanotubes; fullerenes; nanoparticles; electron microscopy; nano-reactors

Our research is focused on the chemistry and materials science of carbon nanostructures and their hybrid composites with organic, inorganic and organometallic compounds. We view a carbon nanostructure as a physical bridge between the world of molecules and the macroscopic world around us. For example, carbon nanotubes, having two of their dimensions at the nanoscale and one dimension at the macroscopic scale, can serve as containers for a wide range of molecules. In 2011, we expanded nano-container applications of carbon nanotubes to new classes of compounds, including organometallic and coordination derivatives of fullerene C_{60}, complex endohedral fullerenes functionalised with organic groups and single-molecules magnets $Mn_{12}Ac$ (in collaboration with Dr. Gimenez-Lopez). Individual atoms of transition metals have been shown to act as catalytic centres inside nano test tubes, promoting unprecedented transformation of guest-molecules and, in some metals, reacting with the inner surface of host-nanotube. Up to now, the chemical reactivity of the nanotube interior was considered to be non-existent, but our methodology discovered a range of new chemical reactions imaged at the atomic level by low-voltage aberration corrected transmission.

We have demonstrated that nanotubes can be utilised as efficient nano-reactors and 1D templates leading to the formation of new, unexpected products. One of the most unusual reactions is the transformation of organic molecules into graphene nanoribbons. Nanoribbons are usually unstable, but we have shown that termination of edges with sulphur atoms leads to thermodynamically stable 1D nanostructures, which exhibit interesting dynamic behaviour inside nanotubes. Latest developments in the area of fullerenes include new optically- and redox-active fullerene conjugates with polyaromatic molecules, which have been demonstrated as highly efficient electron acceptor systems, and the first example of controlled assembly of fullerenes into molecular monolayers (SAMs) guided by the structure of thiol/thioether group attached to the fullerene surface.

Highlight publications

Chuvilin, A., Bichoutskaia, E., Gimenez-Lopez, M. C., Chamberlain, T. W. Rance, G. A., Kuganathan, N., Biskupek, J., Kaiser, U., and Khlobystov, A. N. (2011) Self-assembly of a sulphur-terminated graphene nanoribbon within a single-walled carbon nanotube. Nature Mat.10, 687-692

Chamberlain, T. W., Meyer, J. C., Jannik J. Biskupek, J. Leschner, J., Santana, A., Besley, N. A., Bichoutskaia, E., Kaiser, U., and Khlobystov, A. N. (2011) Reactions of the inner surface of carbon nanotubes and nanoprotrusion processes imaged at the atomic scale. Nature Chem. 3, 732-737.

Dr Pete Licence

Ionic Liquids; ultra-high vacuum, X-ray photoelectron spectroscopy (XPS); electrochemistry; catalysis; materials; physical organic chemistry

The Nottingham ionic liquids research group is an interdisciplinary group active at the interface between inorganic and physical chemistry. Our principle interests evolve around the structure and reactivity of interfaces and phase boundaries and the impact that they can have of catalysis and materials processing. Because they are composed entirely of ions, ionic liquids have almost zero vapour pressure and do not evaporate even under vacuum. Over the past 5 years, we have developed a range of UHV based experimental methods and used X-ray Photoelectron Spectroscopy (XPS) to characterise a wide range of ionic liquid based systems. In early 2011 we published a landmark paper in the RSC journal PCCP that described a series of experiments, which have defined charge referencing during the measurement of XP spectra in ionic liquids. This method has been central to the communication of preliminary results of ongoing projects including the investigation of anion-cation interactions in pure ionic liquids and the study of solute-solvent interactions in ionic liquid based solutions that find application in homogeneous catalysis and energy related systems including dye sensitised solar cells, ion selective electrodes and batteries.

In addition to spectroscopic projects involving UHV spectroscopy, our group has also pioneered the use of UHV in liquid-phase synthetic chemistry. The unusual BF_3 and PF_5 bonded imidazol-2-ylidenes (left) are prepared in a remarkably high yield (> 95 %) from a precursor ionic liquid in just a single step. The materials form crystalline solids which are remarkably stable and are currently under investigation for NLO properties.

Highlight publications

Puttick, S., Davis, A. L., Butler, K., Lambert, L., El harfi, J., Irvine, D. J., Whittaker, A. K., Thurecht, K. J., and Licence, P. (2011) NMR as a Probe of Nanostructured Domains in Ionic Liquids: Does Domain Segregation Explain Increased Performance of Free Radical Polymerisation? Chem. Sci. 2, 1810-1816

Villar-Garcia, I. J., Smith, E. F., Taylor, A. W., Qiu, F., Lovelock, K. R. J., Jones, R. G., and Licence, P. (2011) Charging of Ionic Liquid Surfaces Under X-ray Irradiation: The Measurement of Absolute Binding Energies by XPS. Phys. Chem. Chem. Phys. 13, 2797-2808

Dr Steve Liddle

f-element chemistry; organometallic chemistry; uranium; rare earths; small molecule activation; nanomagnetism

Research in the Liddle group concerns all aspects of molecular f-element chemistry, with particular emphasis on metal-metal bonding and reactivity, metal-ligand multiple bond linkages such as carbenes, small molecule activation, and nanomagnetism. We target complexes which challenge preconceived ideas about structure, bonding, and reactivity and complementary structural, spectroscopic, magnetometric, and computational methods are routinely employed to understand new compounds.

Our studies of metal-metal complexes target unsupported uranium-transition metal bonds. Our focus is to isolate complexes in which there is a direct covalent bond between uranium, which may engage in bond metathesis reactions, and transition metals which readily engage in redox chemistry. This is in order to understand the bonding that uranium is capable of undertaking and to unlock designed synergic reactivity for the activation of small molecules of industrial relevance such as carbon monoxide, carbon dioxide, and methane.

Our studies of metal-ligand multiple bond linkages has led us to establish a programme that is systematically examining the nature and reactivity of f-element carbenes which contain a covalent metal-carbon double bond. We can demonstrate regioselective C-H activation and subsequent C-C/C-O bond formation chemistry which generates complex organic molecules in one pot. This work has also resulted in the realisation that these compounds can form the basis of single molecule magnets which derive their magnetism from molecular rather than bulk properties and which are attractive candidates for quantum computing and ultra-high-density data storage.

Highlight publications

Cooper, O. J., Mills, D. P., McMaster, J., Moro, F., Davies, E. S., Lewis, W., Blake, A. J., and Liddle, S. T. (2011) Uranium-Carbon Multiple Bonding: Facile Access to the Pentavalent Uranium Carbene $[U\{C(PPh_2NSiMe_3)_2\}(Cl)_2(I)]$ and Comparison of U^{V}=C and U^{IV}=C Double Bonds. Angew. Chem. Int. Ed. 50, 2383-2386

Mills, D. P., Moro, F., McMaster, J., van Slageren, J., Lewis, W., Blake, A. J., and Liddle, S. T. (2011) A delocalised arene-bridged diuranium single molecule magnet. Nat. Chem. 3, 454-460

Prof Barry Lygo

Asymmetric catalysis; phase-transfer catalysis; natural product synthesis; synthetic methodology; application of computational methods in catalyst design

Single enantiomer molecules are widely employed in pharmaceutical/biomedical research and over half of the worldwide-approved drugs are now single enantiomers. The most versatile and efficient means of producing single-enantiomer building blocks is via asymmetric catalysis, and in recent years there has been an explosion of interest in the use of chiral small organic molecule catalysts (organocatalysts) for this purpose. Catalysts of this type have many attractive features:

- they can be used to promote a wide range of chemical transformations
- they can be used under mild reaction conditions (aqueous environment, ambient temperature and pressure)
- the catalysts can be inexpensive, non-toxic, and biodegradable

Unfortunately few catalysts of this type are currently suitable for use on industrial scale. This is because most of the processes developed so far require high catalyst loading (10-30 mol %), long reaction times (several days), and a large excess of one reagent. In order to help realize the true potential of this methodology we seeking to develop far more efficient organocatalyst structures. Current research projects in this area include:

- development of new and improved organocatalysed asymmetric processes for the preparation of key pharmaceutical and agrochemical intermediates
- development of reliable computational methods for catalyst design and optimisation
- application of asymmetric PTC alkylation in the synthesis of complex amino acid and alkaloid natural products

In recent years this work has resulted in the development of highly enantioselective phase-transfer alkylation and epoxidation processes that only require 0.1-1 mol% catalyst, and deliver key synthetic intermediates with high enantioselectivity. This year we have successfully developed a simple diamine catalyst that is capable of promoting highly diastereo- and enantioselective aldol reactions using as little as 3 mol% catalyst.

Highlight publications

Lygo, B., Davison, C., Evans, T., Gilks, J. A. R., Leonard, J., Roy, C. -E. (2011) Highly Enantioselective Aldol Reactions Using Tropos Dibenz[c,e]azepine Organocatalysts. Tetrahedron 67, 10164-10170

Lucas, C. L., Lygo, B., Blake, A. J., Lewis, W., Moody, C. J. (2011) Regioselectivity of the Claisen Rearrangement in meta-Allyloxy Aryl Ketones: An Experimental and Computational Study, and Application in the Synthesis of (R)-(-)-Pestalotheol D. Chem. Euro. J. 7, 1972-1978

Dr Jonathan McMaster

Bioinorganic chemistry; co-ordination chemistry; EPR spectroscopy; MCD spectroscopy; DFT calculations

Research in the McMaster group focuses on the roles of d-transition metals in biology. The recent progress in protein X-ray crystallography and spectroscopy has lead to detailed static pictures for the structures of the active sites of numerous metalloproteins. As a result, a major challenge for the bioinorganic chemist is to understand the properties and functions of metalloenzymes within this well-defined structural framework. Ultimately, insight into the properties of biological metal centres derives from a description of the electronic structure of the active site and how other enzyme motifs perturb it.

The McMaster Group is currently engaged in:

- the development of analogues of the active sites of the [NiFe] hydrogenases as potential catalysts for the production of dihydrogen
- the preparation of metal complexes of novel sterically hindered ligands capable of supporting thiyl or phenoxyl radicals bound to transition metal centres
- understanding the mechanism of electron transfer between the prosthetic groups in the Mo-containing hydroxylases and oxotransferases, deriving an electronic structure description for the molybdenum cofactor in the Mo-containing hydroxylases and oxotransferases through spectroscopic studies of Mo and W complexes with S ligands
- the use of electrochemical methods, electron paramagnetic and magnetic circular dichroism spectroscopies and theoretical calculations to probe the electronic structures of transition metal compounds

Highlight publications

Whalley, A. L., Blake, A. J., Collison, D., Davies, E.S., Disley, H.J., Helliwell, M., Mabbs, F.E., McMaster, J., Wilson C., and Garner, C.D. (2011) Synthesis, structure and redox properties of bis(cyclopentadienyl)dithiolene complexes of molybdenum and tungsten, Dalton Trans. 40, 10457-10472

Stephen, E., Huang, D.G., Shaw, J. L., Blake, A. J., Collison, D., Davies, E. S., Edge, R., Howard, J. A. K., McInnes, E. J. L., Wilson, C., Wolowska, J., McMaster, J., and Schröder, M. (2011) Redox Non-Innocence of Thioether Crowns: Spectroelectrochemistry and Electronic Structure of Formal Nickel(III) Complexes of Aza-Thioether Macrocycles. Chem.-Eur. J. 17, 10246-10258

Prof Robert Mokaya

Porous materials; solid state chemistry; supramolecular templating; Energy storage; Nanomaterial fabrication; Heterogeneous catalysis

The design, synthesis and characterisation of novel porous materials and the study of their structure-property relations is the focus of our research interests. The materials currently under investigation are those that may find use as solid state catalysts, adsorbents, molecular sieves, energy stores and as hosts in the preparation of advanced composite materials.

Our research therefore spans the areas of heterogeneous catalysis, molecular sieving, sustainable energy materials and host/guest chemistry. Of particular interest are structurally well ordered porous solids such as zeolites, pillared layered materials, mesoporous molecular sieves and carbons of various forms.

Specific research themes include; (i) the development of new micro or mesoporous solid-state catalyst, (ii) tailoring and morphological control of porous silicates and carbons, (iii) carbon-based nanostructures as hydrogen and CO_2 stores, and as electrode materials for supercapacitors.

Highlight publications

Wei, L., Sevilla, M., Fuertes, A. B., Mokaya, R., and Yushin, G. (2011) Hydrothermal Carbonization of Abundant Renewable Natural Organic Chemicals for High-Performance Supercapacitor Electrodes. Adv. Energy Mater., 1, 356–361

Masika, E., and Mokaya, R. (2011) Mesoporous aluminosilicates from a zeolite BEA recipe. Chem. Mater. 23, 2491–2498

Prof Christopher J Moody

Organic chemistry; medicinal chemistry

Research interests span organic chemistry and include synthetic methodology, synthesis of bioactive natural products, and medicinal chemistry. In synthetic methodology we are interested in the application of transition-metal catalysed carbene X-H insertion reactions in new approaches to important heterocyclic molecules, in new applications of the Claisen rearrangement, and in oxidative processes in synthesis.

Nature continues to provide us with challenging structures to test our ideas about chemical reactivity and synthesis. Natural products have fascinating and complex structures that have been evolutionary selected over millions of years, and therefore often have interesting medicinal properties. We are interested in the synthesis of a number of biologically active marine and terrestrial natural products.

Many natural products possess powerful medicinal properties, and these can be used to guide the synthesis of potentially useful analogues for the treatment of disease. We are particularly interested in anticancer and antimalarial compounds that act by novel mechanisms such as the inhibition of the quinone reductase enzymes (NQO1 and NQO2) and the molecular chaperone Hsp90. Compounds of interest include heterocyclic quinones, macrocyclic lactones and ansaquinones.

Highlight publications

Linder, J., Garner, T. P., Williams, H. E. L., Searle, M.S., and Moody, C. J. (2011) Telomestatin: formal total synthesis and cation-mediated interaction of its seco-derivatives with G-quadruplexes. J. Am. Chem. Soc. 133, 1044-1051

Day, J. E. H., Sharp, S. Y., Rowlands, M. G., Aherne, W., Hayes, A., Raynaud, F. I., Lewis, W., Roe, S. M., Prodromou, C., Pearl, L.H., Workman, P., and Moody, C.J. (2011) Targeting the Hsp90 molecular chaperone with novel macrolactams. Synthesis, structural, binding and cellular studies. ACS Chem. Biol. 6, 1339-1347

Dr John Moses

Natural product synthesis; synthetic methodology; biomimetic synthesis; click chemistry

Research in the Moses group is focussed upon the common theme of Biomimetic Chemical Systems, following Nature's guiding principles. Projects are split into complementary areas based around core organic chemistry:

Biomimetic Synthesis — developing complexity generating reactions to facilitate the syntheses of complex natural products.

Click Chemistry — developing new high energy 'click' reactions for application in synthesis and drug discovery.

Drug Discovery — design and synthesis of natural product based drugs employing biomimetic diversity oriented synthesis and click chemistry principles: We are keen to exploit our developed methodologies for the synthesis of new biologically active molecules with potential therapeutic application.

Chemical Biology — design and application of biomimetic systems: Our efforts in this area have focussed on three projects (i) G-quaduplex DNA based asymmetric catalysis. We have described the first tuneable and modular DNA based catalyst using higher order DNA structures, and demonstrated its application in the asymmetric Diels-Alder reaction (ii) Developing molecular probes and tools for the study of biology.

Highlight publications

Sharma, P., Ritson, D. R., Burnley, J., and Moses, J. E. (2011) A Synthetic Approach to Kingianin A Based Upon Biosynthetic Speculation. Chem. Commun. 47, 10605-10607

Moorhouse, A. D., Spiteri, C., Sharma, P., Zloh, M., and Moses, J. E. (2011) Targeting Glycolysis: A Fragment Based Approach Towards Bifunctional Inhibitors of hLDH-5. Chem. Commun. 47, 230-232

Dr Neil Oldham

Biomolecular mass spectrometry; ion mobility spectrometry; non-covalent protein complexes; protein conformation; protein post translational modifications

My main research interests lie in the application of mass spectrometry in studying biomolecular structure and interactions. Areas of particular activity are the investigation of non-covalent protein complexes, and the characterisation of protein (post translational) modification.

Notable results over the last year include the first detection of a dynamic equilibrium between enzyme conformers using ion mobility spectrometry and mass spectrometry, the discovery of destabilisation of protein-ligand complexes in the gas phase by alkali metal ion adduction, and the development of a method for charge state and adduct reduction of in electrospray ionisation. The latter development has proved particularly beneficial in stabilising weak protein complexes and overcoming the destabilising effects of alkali metals.

Highlight publications

Hopper, J. T. S., and Oldham, N. J. (2011) Alkali Metal Cation-Induced Destabilization of Gas-Phase Protein-Ligand Complexes: Consequences and Prevention. Anal. Chem. 83, 7472-7479

Jenner, M., Ellis, J., Huang, W. -C., Lloyd Raven, E., Roberts, G. C. K., and Oldham, N. J. (2011) Detection of a Protein Conformational Equilibrium by Electrospray Ionisation-Ion Mobility-Mass Spectrometry. Angew. Chem. Int. Ed. 50, 8291-8294

Prof Martyn Poliakoff CBE FRS

Green Chemistry; Supercritical Fluids; Continuous Reactions; High Pressure Chemistry; Process Monitoring; Public Engagement - YouTube

Green Chemistry aims to find cleaner, more sustainable processes for making chemicals and materials. My group is interested in replacing the organic solvents traditionally used in such processes by highly compressed CO_2 or H_2O, so-called supercritical fluids. In particular, we have been developing the use of continuous reactors for both heterogeneous and homogeneous catalysis. In recent years, our chemistry has focussed increasingly on reactions of compounds that can be obtained from renewable feedstocks derived from biomass. The research involves extensive collaboration with colleagues in the School of Chemistry and also in the Engineering Faculty and many of the projects include close partnership with industry.

Scientific highlights in 2011 include an investigation into the feasibility of using CO_2 from Carbon Capture and Storage to reduce the energy costs of supercritical hydrogenation; the development of a new IR approach to measuring the phase behaviour of high pressure fluids where a single sensor can detect two different transitions; the discovery that there is a strong synergy in the catalytic action of Cu_2+ and Co_2+ in the industrially important oxidation of para-Xylene to terephthalic acid in supercritical water; and the development of self-optimizing reactors for supercritical CO_2 which reduce the optimisation time for new reactions from months to days.

Our group also plays a leading role in the website, The Periodic Table of Videos www.periodicvideos.com, which has become one of the leading science channels on YouTube. The number of its subscribers across the world passed 60,000 on 30 December and its most popular video has been watched by ca. 580k. In 2011, it was the subject of invited papers in Nature Chemistry and Science as well as featuring in the 2012 Guinness World Records!

Highlight publications

Pérez, E., Fraga-Dubreuil, J., García-Verdugo, E., Hamley, P. A., Thomas, M. L., Yan, C., Thomas, W. B., Housley, D., Partenheimer, W., and Poliakoff, M. (2011) Selective Aerobic Oxidation of para-Xylene in Sub- and Supercritical Water. Part 1: Comparison with ortho-Xylene and the Role of the Catalyst. Green Chem 13, 2389-2396

Pérez, E., Fraga-Dubreuil, J., García-Verdugo, E., Hamley, P. A., Thomas, M. L., Yan, C., Thomas, W., B., Housley, D., Partenheimer, W., and Poliakoff, M. (2011) Selective Aerobic Oxidation of para-Xylene in Sub- and Supercritical Water. Part 2: The Discovery of Better Catalysts. Green Chem. 13, 2397-2407

Prof Ivan Powis

Photoionization Dynamics; Photoelectron Circular Dichroism; Chirality; Vector Correlations; Photodissociation Dynamics

We are interested in studying the dynamics of electrons in polyatomic molecules by observing, in 3D, the nature and probability, excitation, speed and angular distribution of fragments ejected following photo-excitation. This then portrays the forces and torques that have been experienced and exerted in the evolving electronic structure of the molecular species. We further enhance this information using fully variable polarization of the photon sources (synchrotron radiation for SXR–VUV, lasers for VUV–UV) to control the energy and angular momentum deposited into the molecular target.

In recent years, we have pioneered the development, both theoretical and experimental, of a novel chiroptical technique, photoelectron circular dichroism (PECD), that displays chiral asymmetries of unprecedented magnitude. This unrivalled sensitivity makes it possible to use cold molecular beams in order to achieve spectroscopic and structural measurements with natural products and pre-biotic molecules in solvent-free environments. Recently, these isolated-molecule techniques have been extended to allow the study of small homogeneous chiral clusters and micro-solvated systems, addressing topics including induced chirality in solvent shells and chiral molecular recognition phenomena.

Highlight publications

Powis, I. (2011) Initial-state and final-state vibrational effects in the treatment of molecular photoionization dynamics. Phys. Rev. A 84, 013402

Daly, S., Powis, I., and Garcia, G. A. (2011) Soldi-Lose H, Nahon L. Photoionization of epichlorohydrin enantiomers and clusters studied with circularly polarized VUV radiation. J. Chem. Phys. 134, 064306

Prof Katharine L Reid

Time-resolved ultrafast photoelectron imaging; dynamics of excited state molecules

We develop and use laser photoelectron imaging techniques, including ultrafast time-resolved techniques, to investigate structure and mechanisms of intramolecular energy redistribution in the excited states of small polyatomic molecules. Our ultrafast experiments are conducted with a unique laser system that produces pulses of 1 ps in duration, sufficiently short to monitor many intramolecular dynamical processes, but which have a spectral profile that enables the resolution of vibrational structure, and sometimes torsional structure, in small aromatic molecules. This capability, used in conjunction with novel methods of detection and analysis, has allowed us to quantitatively determine the coupling matrix elements that drive some of the energy redistribution processes in toluene and p-fluorotoluene.

We are also developing techniques that enable us to use the photoelectron angular distributions derived from our photoelectron images to provide structural information on small polyatomic molecules. For example, in recent work we have shown that we can obtain photoelectron angular distributions corresponding to individual rotationally resolved levels in light polytomic molecular ions, and that the complicated three-dimensional photoelectron angular distributions that arise in the frame of an individual molecule can be tomographically reconstructed from carefully designed measurements.

Highlight publications

Davies, J. A. and Reid, K. L. (2011) Intramolecular vibrational dynamics in S_1 p-fluorotoluene. I. Direct observation of doorway states. J. Chem. Phys. 135, 124305

Dr David Robinson

Electronic excited states, CASSCF, TDDFT, MD, fluorescence, membranes

My research focuses on the nature of biological (cell) membranes and the information we can retrieve by using fluorescent probes. Experimental methods have given lots of data, for which theoretical methods can garnish with atomistic detail. I have shown that the most commonly employed membrane probe, di-8-ANEPPS, has fluorescence shifts dictated only by the electrostatic nature of a membrane and not specific molecular interactions. I am further refining the molecular dynamics (MD) force-fields to include the effects of electronic polarisability explicitly.

Highlight publications

Robinson, D., Besley, N. A., O'Shea P., and Hirst, J. D. (2011) Water Order Profiles on Phospholipid / Cholesterol Membrane Bilayer Surfaces. J. Comp. Chem. 32, 2613-2618

Robinson, D., Besley, N. A., O'Shea, P. and Hirst, J. D. (2011) Di-8-ANEPPS Emission Spectra in Phospholipid/ Cholesterol Membranes: A Theoretical Study. J. Phys. Chem. B 115, 4160-4167

Prof Peter Sarre

Astrochemistry; spectroscopy; telescope; interstellar molecules; molecular astrophysics; computational chemistry

The Astrochemistry Group undertakes observational, modelling and laboratory spectroscopic-based research at the interface of chemistry, physics and astronomy. Current areas of interest cover ultraviolet, visible and infrared studies of molecules and dust in interstellar, nebular, circumstellar and stellar media.

The single largest project is research into the problem of the `diffuse interstellar absorption bands' which have remained unidentified since the first was discovered almost 100 years ago. We conduct research on a wide variety of other exciting topics including the 'Unidentified' IR Emission Bands believed to be due to polycyclic aromatic hydrocarbons, carbon molecules in cool stars and young stellar objects, and the small-scale structure and chemical composition of the interstellar medium. Our laboratory studies are focussed on the catalytic formation of large aromatic molecules on silicate grain surfaces and electronic spectroscopy of short-lived large carbon-based molecules.

The Group has been awarded observing time on a range of telescopes including the William Herschel Telescope, Gemini South, ESO's Very Large Telescope, the Southern African Large Telescope, the Herschel satellite and most recently on NASA/DLR's Stratospheric Observatory for Infrared Astronomy (SOFIA) – a converted high-flying Boeing 747 SP jet with a telescope aboard.

Highlight publications

Cordiner, M. A., Cox, N. L. J., Evans, C. J., Trundle, C., Smith, K. T., Sarre, P. J and Gordon, K. D. (2011) A survey of diffuse interstellar bands in the Andromeda Galaxy: optical spectroscopy of M31 OB stars. Astrophys. J. 726, 39-50

Garkusha, I., Fulara, J. Maier, J. P. and Sarre, P. J. (2011) Electronic Absorption Spectra of Protonated Pyrene and Coronene in Neon Matrices. J. Phys. Chem. A. 115, 10972-10978

Prof Martin Schröder

Coordination chemistry; nanomaterials discovery; fuel gas storage and selectivity; hydrogen storage and production; metalloanion and cation binding and sequestration

Our research interests span the co-ordination, organometallic and supramolecular chemistry of metal complexes targeting applications across energy and sustainability research. The design, synthesis and understanding of chemical function and of binding and recognition of substrates are underpinned by fundamental studies in ligand design, complex synthesis and characterisation. Our research focuses on the following areas:

Porous Metal-Organic Frameworks — metal-organic frameworks (MOFs) are coordination polymers incorporating permanent porosity that can be used to store and separate gas and liquid substrates. We have prepared a range of porous materials that show particularly high storage capacities for H_2 and, depending upon the system, interesting and varying selectivities between CO_2, CH_4, H_2, N_2, O_2 and SO_2. Cation exchange in anionic framework materials has led to materials that show hysteretic and gated gas uptake characteristics, and state-of-the-art structural characterisation of gas-loaded materials has afforded vital information how these dynamic materials interact with substrates.

Catalysts for Hydrogen Production — hydrogenase enzymes incorporate multi-metal sites that interconvert reversible H_2 and protons (H^+). We have successfully prepared NiFe complexes that mimic the active site of these metalloenzymes and have confirmed their ability to reduce protons to H_2 under electrochemical conditions. Current work seeks to achieve this photocatalytically using visible light that is absorbed by a photosensitizer which relays electrons to the catalytic centre.

Cation and Anion Binding and Sequestration —the binding of metal cations and anions to macrocyclic and open chain ionophores represent a route to the clean extraction and transport of toxic and precious metal values. Ionophores and receptors for metal salt extraction and transport have been developed and their ability to bind different metal salts modulated via ligand design and the incorporation of hydrogen and halogen bonding moieties.

Highlight publications

Tan, C., Yang, S., Lin, X., Blake, A. J., Lewis, W., Champness, N. R., and Schröder, M. (2011) High Capacity Gas Storage by a 4,8-Connected Metal-Organic Polyhedral Framework. Chem. Comm. 47, 4487-4489

Yan, Y., Yang, S., Blake, A. J., Lewis, W., Poirier, E., Barnett, S. A., Champness, N. R., and Schröder, M. (2011) A Mesoporous Metal-Organic Framework Constructed from a Nanosized C_3-Symmetric Linker and $[Cu_{24}(isophthalate)_{24}]$ Cuboctahedra. Chem. Comm. 47, 9995-9997

Prof Mark S Searle

Non-covalent interactions in biomolecular recognition; NMR structural biology and biophysics

Research in the Searle group is based around the application of structural and biophysical methods to probe biomolecular interactions relevant to cell signalling pathways, autophagy mechanisms translational regulation, drug-targeted DNA and RNA interactions, specificity in protein-ligand binding and in understanding protein folding pathways. Based in the Nottingham Centre for Biomolecular Sciences (CBS), the research is highly interdisciplinary and involves collaborations with a number of Schools across the biological and medical sciences in Nottingham. The group uses high-field NMR (600 MHz and a new 800 MHz instrument with cryoprobe facilities) and biophysical tools, including isothermal titration calorimetry, CD spectroscopy, ESI mass spectrometry and X-ray crystallography, in collaboration with groups in Chemistry and CBS. Current studies have focused on large multi-domain proteins and their multi-complex assemblies with protein and RNA targets to develop a fundamental understanding of cellular biochemistry, with links to human disease and potential drug-targeting.

The last 12 months have seen significant progress in the understanding of the regulation of mRNA function by the multi-domain CELF1 family of RNA binding proteins which target the 3'-untranslated region of mRNA sequences rich in UGU binding sites, with links to muscular dystrophy and aging. We have also structurally characterised a novel post-transcriptional regulator from the opportunistic human pathogen Pseudomonas aeruginosa and shown how it targets RNA sequences with a GGA recognition site in regulating the translation of a large number of genes required for bacterial survival and host invasion. The proteins p62 and NBR1 are scaffold proteins which play key roles in cell signalling and autophagy degradation mechanisms, with human diseases linked to dysfunctional regulation of their ability to recognise distinct interaction faces of ubiquitin-tagged substrates. P62 and NBR1 form multi-protein interactions whose affinities are further regulated by a number of post-translational modifications which are currently under investigation. The range of structural and biophysical methods is complemented by computational approaches for structural modelling, and molecular biology facilities for protein expression. The majority of the research is funded through the BBSRC.

Highlight publications

Edwards, J., Malaurie, E., Kondrashov, A., Long, J., de Moor, C., Searle, M. S., Emsley, J. (2011) Sequence determinants for the tandem recognition of UGU and CUG rich RNA elements by the two N terminal RRMs of CELF1. Nucleic Acids Res. 39, 8638-8650

Garner, T. P., Strachan, J., Shedden, E. C., Long, J. E., Cavey, J. R., Layfield, R., Searle, M. S. (2011) Independent interactions of ubiquitin-binding domains in a ubiquitin-mediated ternary complex. Biochemistry 50, 9076-9087

Prof Panos Soultanas

Bacterial DNA replication, replication initiation mechanisms, replication-transcription collisions, DNA repair, molecular motors, helicases, primases, protein-protein and protein-DNA interactions

Our interests lie in the broad area of bacterial DNA replication with emphasis on molecular mechanisms of replication initiation, helicase and primase activities, replication-transcription collisions and DNA repair. Our work on replication-transcription collisions has featured in the spring 2011 edition of the BBSRC Business magazine where the BBSRC Chief Executive Prof. Douglas Kell commented that “the interplay between gene expression, DNA replication and the prevention of DNA damage is an example of a tenet of Biology with key ideas, tools, techniques and processes that are applied across an enormous range of topics and has the potential to touch on research right across BBSRC’s portfolio and beyond".

Our studies on the NMR structure of the DNA-interacting C-terminal domain of the essential replication initiation protein DnaD in collaboration with Jeremy Craven (Sheffield) revealed an intrinsically unstructured C-terminus part of which, together with helices H3, H4 and H5, forms the DNA binding module. A strictly conserved YxxxIxxxW motif was discovered in all DnaD-like proteins and a previously unknown structural homology with the replication initiation protein DnaB was discovered.

We have recently discovered that the DNA untwisting activity of DnaD stimulates the DNA repair activity of the Nth endonuclease during abasic site (AP) DNA repair in B. subtilis. The activity of Nth is instrumental during the response to H2O2-induced oxidative damage as an nth gene deleted B. subtilis strain was more sensitive to H_2O_2 exposure.

Highlight publications

Soultanas, P. (2011) The replication-transcription conflict. Transcription 2, 140-144

Merrikh, H., Machón, C., Grainger, W. H., Grossman, A. D., and Soultanas, P. (2011) Co-directional replication-transcription conflicts lead to replication restart. Nature 470, 554-557

Prof Anthony J Stace FRS

Spectroscopy and chemistry of metal dication complexes in the gas phase; theory of how highly charged particles of dielectric materials interact

Developments in experimental technique have made it possible to generate in the gas phase dication complexes consisting of solvated metal ions, $[M(L)_n]^{2}$+. Since these ions are in the gas phase, they offer a unique opportunity to explore topics in spectroscopy, coordination and chemistry that cannot be investigated in the condensed phase because of the presence of bulk solvent and counter ions. To study the spectra of these ion complexes, a quadrupole ion trap apparatus has been developed for recording photofragment spectra from cold metal dication complexes. The apparatus has been adapted to store and cool ions via collisions with a helium buff gas that maintains contact with a liquid N_2 reservoir and the ions appear to achieve internal temperatures of 100-150 K. UV photofragmentation spectra have now been recorded for a number of $[M(pyridine)_4]^{2+}$ and $[M(benzene)_2]^{2+}$ complexes, and in conjunction with DFT, it has been possible to identify transitions between individual electronic states.

Very recently, we made the first experimental observation of where a molecular dication cluster of a single size undergoes metastable Coulomb fission. The results showed a delayed and highly asymmetric fragmentation process (~ 10^{-4} s). To interpret the unexpected fragmentation patterns, the first analytical solution to the problem of how charged particles of dielectric materials interact has been presented. A completely unexpected result from the calculations is that they show how particles carrying the same sign of charge can be attracted to one another; an effect that arises from a mutual polarisation of charge density on the surfaces of particles. In the longer term, the theory has significant implications for the behaviour of charged particles in such diverse areas as the coalescence of water droplets in clouds (charge scavenging), the performance of laser printers (electrophotography), and the delivery of respiratory (tribocharged) drugs from nebulisers.

Highlight publications

Stace, A. J., Boatwright, A. L., Khachatourian, A., and Bichoutskaia, E. (2011) Why Like-Charged Particles of Dielectric Materials can be Attracted to One Another. J. Coll. Interface Sci. 354, 417-420

Wu, G., Chen, X. J., Stace, A. J., and Linse, P. (2011) Delayed Asymmetric Coulomb Fission of Molecular Clusters: Application of a Dielectric Liquid-drop Model. J. Chem. Phys. 134, 031103

Dr Rob A Stockman

Natural product synthesis; synthetic methodology; diversity oriented synthesis; sulfinimine chemistry

Our group’s research is concerned with developing new synthetic methods and strategies which are able to generate molecular complexity in a very short manner, and thus provide quicker methods for the synthesis of high value complex molecules. We have published a number of papers on the synthesis and utility of chiral S-mesitylsulfinimines over the past year. We have found that chiral mesitylsulfinimines offer excellent levels of stereocontrol upon reaction with Grignard reagents and carbenoids, and further we have developed a facile one-pot synthesis of these useful synthetic intermediates. We later took this forward a step further and developed a simple, one-pot synthesis of chiral amines.

Another major theme of the groups research is the development of a unique strategy for the synthesis of complex molecules which combines two-directional synthesis (for the formation of linear chain compounds with reactive functionality at each terminus and at the centre of the chain), and tandem reactions, which are able to “tie up” the long-chained compound, creating several bonds and stereogenic centres, thus creating a complex molecular structure from a simple linear one. This year we have reported on this tactic for the rapid assembly of an advanced precursor of the natural product, halichlorine. We have also developed the two-directional synthesis / tandem reaction strategy for the formation of twelve natural-product-like scaffolds from a sinlge precursor in an average step-count of just 1.25 steps per scaffold.

Rapid access to a range of molecular scaffolds is essential for fragment-based drug discovery, and thus as a proof-of-concept that our approach is able to access very rapidly chemical space relevant to biological activity, we took one of the scaffolds produced and synthesised a small library, which we were pleased to find had several members with significant activity against several cancer cell lines.

Highlight publications

Roe, C., Hobbs, H. and Stockman, R. A. (2011) One-Pot Synthesis of Chiral Non-Racemic Amines. J. Org. Chem. 22, 9452-9459

Robbins, D., Newton, A. F., Gignoux, C., Legeay, J. -C., Sinclair, A., Rejzek, M., Laxon, C. A., Yalamanchili, S. K., Lewis, W., O'Connell, M. A., and Stockman, R. A. (2011) Synthesis Of Natural-Product-Like Scaffolds In Unprecedented Efficiency Via A 12-Fold Branching Pathway. Chem. Sci. 2, 2232-2235

Dr Wim Thielemans

Materials from renewable sources, renewable nanoparticles, aerogels, nanoparticle self-assembly, surface-activated nanoparticles, nanoparticle-based sensors and electrocatalysts

The work in our group is currently focussed on the surface modification of ribbon-like monocrystalline nanoparticles derived from cellulose and their self-assembly and use in advanced materials such as aerogels, membranes, ion exchange applications, nanocomposites, electrochemical sensors, supercapacitors and electrocatalysts.

The surface modifications we use are varied and depend on the envisaged applications. They include modification with ionic liquids, polymers frown from the surface by controlled surface-initiated polymerisation techniques, electrochemically and catalytically active complexes, fluorescent and UV-active molecules, and large chain molecules.

Highlight publications

Labet, M., and Thielemans, W. (2011) Improving the reproducibility of chemical reactions on the surface of cotton nanocrystals: ROP of ε-caprolactone as a case study. Cellulose 18, 607-617

Eyley, S., and Thielemans, W. (2011) Imidazolium grafted cellulose nanocrystals for ion exchange applications. Chem. Commun. 47, 4177-4179

Prof Neil R Thomas

Bioorthogonal chemistry; coenzymes; biotin, CoA, quantum dot; apoferritin; enzyme; inhibitor; tuberculosis; carbohydrates; biocatalysis

We are a multidisciplinary group using a combination of synthesis, protein engineering and biophysical methods, both to develop new biological probes and enzyme inhibitors, and to modify proteins and enzymes to give them enhanced functionality. In ongoing research we have demonstrated that it is possible to encapsulate highly fluorescent PbS quantum dots inside the protein apoferritin for use as molecular probes in vivo. Human apoferritin proteins have been further engineered to incorporate the un-natural amino acid L-azidohomoalanine that can then be efficiently selectively modified using Cu(I)-catalysed click chemistry.

We have demonstrated that apoferritin coated quantum dots are taken up by breast cancer cell lines 20 times faster than by fibroblasts. Apoferritin and other proteins can be selectively modified by azide and alkyne-bearing biotin analogues we have developed using the enzyme biotin ligase. These analogues can still function as affinity tags with (strept)avidin or allow covalent attachment of fluorophores, MRI probes or other functionality as a post-translational modification. This technology has been patented and licensed to Avidity LLC, Aurora, Colorado with whom we are developing commercial kits.

In other research we have reported new inhibitors of the enzyme UDP-Galp mutase which is essential to the growth of Mycobacterium tuberculosis and in collaboration with Sue Watson and Anna Grabowska in Clinical Sciences, identified some semi-synthetic triterpene analogues with anti-proliferation activity in prostate cancer cell lines.

Highlight publications

Paratha, K., Sadeghi-Khomami, A., Cren, S., Robinson, R. I., Woodward, S., Slowski, K., Berast, L., Zheng, B., Thomas, N. R., and Sanders, D. A. R. (2011) Identification of Novel Inhibitors of UDP-galactopyranose mutase by structure-based virtual screening. Mol. Inform. 30, 873-883

Dr Jeremy J Titman

Spectroscopy and chemistry of metal dication complexes in the gas phase; theory of how highly charged particles of dielectric materials interact

2011 saw the installation of a new Bruker AVIII 600 MHz solid-state NMR spectrometer as part of the University of Nottingham's £2M CiF-funded Centre for High-field NMR based in the Centre for Biomolecular Science. The spectrometer is equipped with a state-of-the-art ultrafast MAS probe spinning at rates up to 65 kHz. Using this new apparatus my research group have been able to design and implement new ultrafast MAS symmetry-based recoupling experiments for measuring $^{1}H - {}^{17}O$ internuclear distances and 1H chemical shift anisotropies.

We have also carried out a comprehensive multi-nuclear NMR study (with Prof. Walker, Division of Energy and Sustainability Research) of the mechanism of the dehydrogenation of nano-structured mixtures of $LiBH_4$ and MgH_2, a promising hydrogen storage system. This included the award of 12 days of magnet time at the UK National 850 MHz Solid-state NMR Facility to record ^{25}Mg NMR spectra. The extra capacity provided by the new spectrometer prompted a number of new collaborative solid-state NMR studies: of crystallinity in pharmaceutical compounds (with Profs. Fischer and Roberts, Pharmacy), of structure in phosphate glasses (with Prof. Rudd and Dr Ahmed, Mechanical, Materials and Manufacturing Engineering) of changing soil chemistry in the arctic permafrost as an indicator of global warming (with Dr Sjogersten, Environmental Sciences), of Li co-ordination in metal organic frameworks (with Prof. Schröder, Chemistry) and of micelle formation in ionic liquids (with Dr Licence, Chemistry and Chemical Engineering).

Highlight publications

Powell, A. S., Stoeva, Z., Smith, R. I., Gregory, D. H., and Titman, J. J. (2011) Structure, stoichiometry and transport properties of lithium copper nitride battery materials: combined NMR and powder neutron diffraction studies Phys. Chem. Chem. Phys. 13, 10641–10647

Yang, S., Martin, G. S. B., Titman, J. J., Blake, A. J., Allan, D. R., Champness, N. R., Schröder, M. (2011) Pore with Gate: Enhancement of the Isosteric Heat of Adsorption of Dihydrogen via Postsynthetic Cation Exchange in Metal-Organic Frameworks Inorg. Chem. 50, 9374–9384

Dr Darren Walsh

Electrochemistry; electrocatalysis; fuel cells; scanning electrochemical microscopy; supercapacitors

Research in the Walsh lab is focused on the development of electrochemical methods and devices. Of particular interest is the development of electrochemical methods for energy conversion and storage, while other projects include the development of electroanalytical techniques such as scanning electrochemical microscopy.

Our work in scanning electrochemical microscopy currently involves the development of novel probes for electrocatalytic studies (left) and the study of electron transfer dynamics in room temperature ionic liquids (RTILs). RTILs are especially interesting targets for electrochemical studies as they are non-volatile and have extremely wide potential windows. Our fundamental studies into electron transfer dynamics in RTILs underpin other projects involving the development of RTIL-based fuel cells.

Our studies in energy conversion focus on the development of novel electrolytes and electrocatalysts for low temperature fuel cells. Of particular interest is the development of non-platinum electrocatalysts for O_2 reduction (the cathode reaction in low temperature fuel cells) and proton-conductive, RTIL-based electrolytes for proton exchange membrane fuel cells.

Highlight publications

Lovelock, K. R. J., Ejigu, A., Loh, S. F., Men, S., Licence, P., and Walsh, D. A. (2011) On the Diffusion of Ferrocenemethanol in Room-Temperature Ionic Liquids: An Electrochemical Study. Phys. Chem. Chem. Phys. 13, 10155-10164

Johnson, L., and Walsh, D. A. (2011) Deposition of Silver Nanobowl Arrays using Polystyrene Nanospheres both as Reagents and as the Templating Material, J. Mater. Chem. 21, 7555-7558

Dr Richard Wheatley

Theoretical chemistry; intermolecular forces; molecular simulation; atoms in molecules; carbon capture

Experimental studies including microwave and electronic spectroscopy are being supported by our new theory in an investigation of the electronic ground and excited states of the NO molecule, NO...atom and NO...molecule complexes. Iterated Stockholder Atoms, developed in this group, are a simple, intuitive and appealing picture of atoms, both visually and mathematically. Originally intended for modelling intermolecular forces, they have also been shown to have a strong relationship to covalent bond order.

Calculations of the molecular interactions in carbon dioxide mixtures (especially containing water), and new methods for calculating thermodynamic and kinetic properties, will be used as input for designing more efficient and safer CO_2 compressors, pipelines and storage locations. The energy partitioning method has recently been developed in this group as a promising way of calculating the density of states, free energies and chemical potentials for single components and mixtures.

Highlight publications

Do, H., Hirst J. D., Wheatley R. J. (2011) Rapid calculation of partition functions and free energies of fluids. J. Chem. Phys. 135, 174105

Oakley, M. T., Do, H., Hirst, J. D. and Wheatley, R. J. (2011) First principles predictions of thermophysical properties of refrigerant mixtures. J. Chem. Phys. 134, 114518

Prof Simon Woodward

Catalysis, selective synthesis, organometallics, C-C bond formation, asymmetric

Our group's current research concentrates on the identification of new compounds and conditions that allow novel (often catalytic) reactions to be carried out that cannot be attained with high efficiency using known chemistry. We aim to employ user-friendly, low cost, environmentally benign reagents in procedures that are simple to carry out.

In a highlight of 2011, Simon Woodward concluded chairing a Europe-wide COST Action covering 23 countries and over 400 scientists that has resulted in publication of a book covering many new concepts in Innovative catalysis.

Highlight publications

Crampton, R., Woodward, S., Fox, M. (2011) Bis-Sulfamyl Imines: Potent Substrates for Asymmetric Additions of Aryl Boroxines under Rhodium-Catalysis. Ad. Synth. Catal. 353, 903-906

Partha, S. K., Sadeghi-Khomami, A., Cren, S., Robinson, R. I., Woodward, S., Slowski, K., Berast, L., Zheng, B., Thomas, N. R., Sanders, D.A.R. (2011) Identification of Novel Inhibitors of UDP-Galactopyranose Mutase by Structure-Based Virtual Screening. Mol. Inform. 30, 873-883

Prof Timothy Wright

Electronic spectroscopy; zero-kinetic-energy (ZEKE) spectroscopy; molecular complexes/clusters; substituted benzenes; quantum chemistry; molecular interactions

Electronic spectroscopy of molecular complexes: We produced molecular complexes in the gas phase at very low internal temperatures, using supersonic free-jet expansion. We have recently been studying the Au-RG complexes (RG = Ne, Ar, Kr and Xe), looking at the electronic spectroscopy and photodissociation behaviour. From this work, we have discovered new electronic states, and observed very complicated photophysical behaviour. In collaboration with a group at Oxford (Dr. Mackenzie), we have derived binding energies for Au-Ar, Au-Kr and Au-Xe, which are to be included in the next edition of the CRC Handbook of Chemistry and Physics. Work on NO–alkane complexes was completed towards the end of the year, and we also were involved in a collaborative project on the assignment of the electronic spectroscopy of $LiNH_3$ with a group (Prof. Ellis) at the University of Leicester.

Interactions in M^+–RG (and other) Complexes: Interactions in the titular species can be weak (<100 cm^{-1}) or very substantial (many 1000s cm^{-1}). An understanding of the evolution of these interactions is essentially a way of viewing the evolution of long-range physical interactions between an ion and a neutral "molecule" through to chemical bond formation. We study these effects using a variety of approaches: an electrostatic model potential; high-level ab initio calculations; wavefunction contour plot analysis; population analysis (such as natural bond order, NBO). We also had the opportunity of completing our work on the Cl –RG complexes, which involved a collaboration with Prof. Kirkpatrick (St. Louis University) and Prof. Viehland (Chatham University).

Zero-kinetic-energy (ZEKE) spectroscopy: This technique uses pulsed-field ionization of high-lying Rydberg states to obtain very high resolution photoelectron spectra. We have been using this to study the vibrational energy levels of the toluene cation ($C_6H_5CH_3$ and $C_6H_5CD_3$). In so doing, we uncovered a wide range of inconsistency regarding the labeling and assignment of the various vibrations (in the ground, first excited singlet and cationic states), and so proposed a new labeling scheme, which we hope will become the standard in the area. In 2012, we shall be recording ZEKE spectra of NO-X complexes and M-X complexes.

Highlight publications

Varriale, L., Bhalla, N., Tonge, N. M., Ellis, A. M., and Wright, T. G. (2011) Near-infrared Spectroscopy of $LiNH_3$: First Observation of the Electronic Spectrum J. Chem. Phys. 134 124304

Gardner, M., and Wright, T. G. (2011) Consistent assignment of the vibrations of monosubstituted benzenes. J. Chem. Phys. 135 114305

Dr Sihai Yang

Solid state chemistry; porous materials; carbon capture; toxic gas capture

Our research aims to develop environmental-friendly strategy to capture harmful gases (e.g. carbon dioxide, sulphur dioxide) at an economically viable cost. We will systematically investigate the processes involved in gas capture by extended porous framework materials, using in-situ structural studies by high resolution synchrotron diffraction and neutron scattering, combined with computational investigations of gas capture process. Microporous materials containing nanosized cavities, the walls of which are decorated with various active sites, can form functional porous traps which are specific to different gas molecules.

Our research aims to determine what happens to the gas molecules inside these materials, and find out how and where the gas molecules interact with the walls of the cavities. Such knowledge will allow the design of successive generations of porous solids with enhanced capabilities to capture and store gases. The programme of research will not only afford significant advances in carbon capture technologies relevant to the development of the 'Low-Carbon Economy', but will also greatly accelerate the pace of development of porous solid adsorbents as viable candidates for selective gas capture and separation.

Highlight publications

Yang, S., Callear, S. K., Ramirez-Cuesta, T. A. J., David, W. I. F., Sun, J., Blake, A. J., Champness, N. R., Schröder, M. (2011) Pore with Gate: Modulating Hydrogen Storage in Metal Organic Framework Materials via Cation Exchange. Faraday Discuss. 151, 19-36

Yang, S., Martin, G. S. B., Titman, J. J., Blake, A. J., Allan, D. R., Champness, N. R., Schröder, M. (2011) Pore with Gate: Enhancement of the Isosteric Heat of Adsorption of Dihydrogen via Post-synthetic Cation Exchange, Inorg. Chem., 50, 9374-9384

RESEARCH

Graduates

We heartily congratulate all our students who graduated in 2011. Many of the undergraduates have progressed onto postgraduate study or into employment in the chemistry-using industries or other gainful employment. Some examples of recent graduate destinations include:

Abercrombie & Fitch; B & V Water Treatment; Bwwank of America Merrill Lynch; Barclays Capital; Biochrom Ltd; BioFocus; Boots; British Telecom; Critical Pharmaceuticals; Custom Pharmaceuticals Ltd; Deloitte; Defence Science and Technology Laboratory; Ernst & Young; Exopack Advanced Coatings; Forensic Science Service; HM Revenue & Customs; Intertek Analytical Services; Lafarge; Local education authorities, (teaching); Lovania; Met Office; Ministry of Defence; National Audit Office; National Health Service; Onyx Scientific; Pegasus Waste Management; PFP Benefit Solutions; Reckitt Benckiser; Research Councils UK; Rolls-Royce; Syngenta; Takeda Cambridge Limited; Unilever

GRADUATES

BSc graduates 2011

Claire Alice Appleby
Jaiya Bhandari
Justyna Bogucka
Taraneh Bozorgzad Moghim
Sean Clancy
Laura Delegate
Thomas James Gibson
Siti Nadiah Ismail
Eric Chee Hong Lim
Sneha Patel
Roslaili Yuhanis Ramli
Saul Robinson
James Rushton
Daniel Adam Simons
Annie Louise Skidmore
Zhi Shan Tan
Carolyn Louise Taylor
Tulsi Vyas
Sophia Evelyn Whitlock
Stephanie Woods
Gregory Simon Plumridge
Paul Smith
Fatimah Aslam
Amarpreet Kaur Dhanoa
Thomas Adam Johnstone
Funminiyi Mosadoluwa Obilanade
Julia Helen Perry
Matthew James Shields
Robert Owen Warren
Nenlepmwa Gofwan Paul
Charles Paul Bentley Heathcote
Sophie Lewis
Laura Elizabeth Mayes
Brogan Simpson
Frances Still

MSci graduates 2011

Name	Dissertation Title	Supervisor
Milan Arambasic	Chiral Brønsted acid catalysis	Prof Chris Hayes
Alexander Ayres	Group ten dimers: potential precursors to the formation of uranium-transition metal monds	Dr Steve Liddle
Joanne Bailey	Investigation of the interaction of EDEN-BP binding domains with RNA	Prof Mark Searle
Laurence Barker	Synthesis and characterization of Au electrocatalysts for O_2 reduction	Dr Darren Walsh
Lawrence Barker	Metal salt reduction using cellulose nanowhiskers	Dr Wim Thielemans
Nigel Bird	High pressure crystallographic studies	Prof Sandy Blake
Martyn Brown	Studies on porous metal-organic framework materials for hydrogen storage	Prof Martin Schröder
Toby Blundell	The stabilisation of low-coordinate transition metal complexes using m-terphenyl ligands	Dr Deborah Kays
Matthew Buckley	An investigation into the physical chemistry of amino acid derived ionic liquids	Dr Pete Licence
William Chung	A nucleophilic catalysis approach towards Claisen rearrangements	Dr Jason Camp
Coby Clarke	The reactive distillations of imidazolium ionic liquids containing BF_4^- and PF_6^- anions	Dr Pete Licence
Oliver Dacosta	Formation of catalytically active palladium nanoparticles using renewable sugars for organic catalysis	Dr Jason Camp
Elizabeth Eaves	Controlled polymerisation in ionic liquids	Dr Derek Irvine
Jack Entwistle	Synthesis of new hLDH-5 inhibitors as anticancer agents	Dr John Moses
Benedict Gilkes	Vibrational analysis beyond the harmonic approximation	Dr Nicholas Besley
Leon Goldney-Sidley	Synthesis of amidinates to stabilise group 2 complexes	Dr Deborah Kays
Matthew Gregson	Synthesis of rare earth carbenes	Dr Steve Liddle
Paul Hamill	Accessing Novel Chiral Sulphonamide N-Heterocyclic Carbenes	Prof Simon Woodward
Liam Higgins	The spectroscopy of blue copper proteins	Dr Nicholas Besley
Rachel Hill	Molecular dynamics of myoglobin	Prof Jonathan Hirst
Sophie Jenkins	Synthetic analogues of the [NiFe] hydrogenase active site	Dr Jonathan McMaster
Christopher Kent	Stereoselective dipolar cycloadditions	Dr James Dowden
Miranda Lowe	Bistable magnetic spin crossover nanoparticles	Dr Andrei Khlobystov Dr Maria del Carmen Gimenez-Lopez
Si Ma	Electrospray ionisation-mass spectrometry applied to protein-interactions	Dr Neil Oldham
Bruce MacNicholl	Synthesis of anticancer indolequinones	Prof Christopher Moody
Amy Middleton-Gear	Synthesis and reactivity of distorted planar four-coordinate carbon centres	Dr Steve Liddle
Scott Miners	Controlled oxidative cutting of carbon nanotubes	Dr Andrei Khlobystov
Ahmed Mohammed	Probing the structural conformation of transglutaminase II with electrospray ionisation ion mobility mass spectrometry	Dr Neil Oldham
Richard Moon	Investigation into the measurement of thermodynamic properties of ionic liquids using a quartz crystal microbalance	Prof Robert Jones
Thomas Murphy	Ionic liquid ultra-thin films at gold single crystal surfaces	Prof Robert Jones
Rasa Mutore	Studies towards the synthesis of magnolignan F	Dr Ross Denton
Ruth Newby	New porous materials derived from M(III) complex nodes	Prof Martin Schröder
Kieron O'Donovan	Study of mechanisms for the formation of endohedral metallofullerenes	Dr Elena Bichoutskaia
Rosalind Onions	Computational modelling of transformation between carbon nanomaterials in transmission electron microscopy	Dr Elena Bichoutskaia
Graham Parkes	The development of a novel photochemical switch	Dr John Moses
James Pegg	Investigating 3+2 cycloadditions: towards total chemical synthesis of securinine	Dr James Dowden
Andrew Pitts	Development of a continuous flow synthesis of sulfinimines and chiral amines	Dr Rob Stockman
Madeleine Pounder	Polycyclic aromatic hydrocarbon molecules in space	Prof Peter Sarre
Adam Prezslak	Diversity oriented synthesis of heterocyclic scaffolds	Dr Rob Stockman
Suzanna Reeves	In-flow use of diazo compounds for heterocycle formation	Prof Chris Hayes
Christopher Reynolds	Stabilising low-coordinate transition metal complexes using sterically demanding m-terphenyl ligands	Dr Deborah Kays
Calum Robertson	Carbon aerogels for carbon dioxide and hydrogen storage	Prof Robert Mokaya
Simone Roloff-Standring	New technologies using azides	Dr John Moses
H. Scarlin	Studies towards the synthesis of chimonanthine and calycanthine	Prof Barry Lygo
Rachael Sellick	Folding of the regulatory RNA-binding proteins RsmA and RsmN	Prof Mark Searle
Aarti Shah	Hydrogen adsorption using porous carbons synthesised from MCM-41 silica template	Prof Robert Mokaya
Andrew Shannon-Little	Studies towards the syntheses of two chlorinated fatty acid targets	Dr Ross Denton
Harry Shirley	A novel noble metal-catalysed glycosylation method	Dr Jason Camp
Geoffrey Smith	Towards the Optimisation of New Stetter Reactions	Prof Simon Woodward
Jasper Smith	Synthesis of novel metal-containing dipyrromethene complexes	Prof Neil Champness Dr Deborah Kays

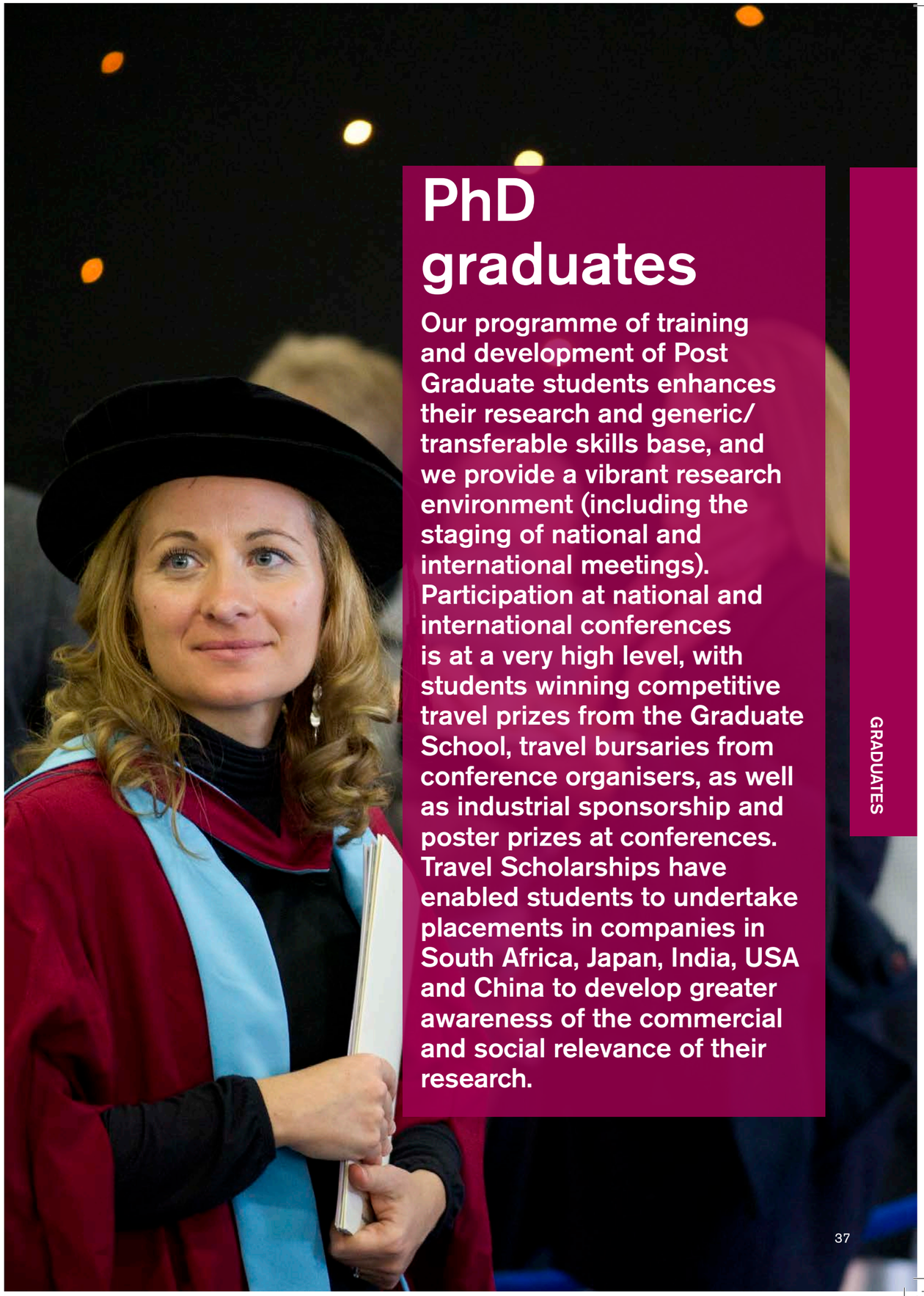
Marcus Smith	Synthesis of the parvistemins	Prof Christopher Moody
C. Starkie	Organocatalyst-based routes to aldol products	Prof Barry Lygo
James Thompson	Photoelectron images from the excited states of small aromatic molecules	Prof Katharine Reid
Hannah Turck	Carbon Nanostructures in the Interstellar Medium?	Prof Peter Sarre
Rachel Wallbridge	Nitroxide-mediated polymerisation from cellulose nanocrystal surfaces	Dr Wim Thielemans
Rebecca Walker	Rapid screening of electrocatalysts using ring-disk ultramicroelectrodes	Dr Darren Walsh
Kate Woodward	Biophysical studies of DNA quadruplexes	Prof Mark Searle
Victoria Wilton	ZEKE Spectroscopy of Toluene-D3 and Interactions in the X1Σ Electronic State of M·RG	Prof Timothy Wright
S. Windle	Development of (S)-proline derived diamine catalysts for the asymmetric aldol reaction	Prof Barry Lygo
Gui Xao	The kinetics of the Cordova asymmetric organocatalytic epoxidation	Dr Ross Denton
Dayang Wahidatu Ashriha binti Awang Haji Ya'akub	Synthesis of functionalized fullerenes for C60X@SWNT peapod formation	Dr Andrei Khlobystov

MSc Chemistry & Entrepreneurship Graduates 2011

Name	Dissertation Title
Jun Qi	Extending CellAura's Offering in the Field of Diagnostics
Robrecht Sean Alexander Van De Giessen	Extending CellAura's Offering in the Field of Diagnostics
Evi Votsi	Evaluating the potential for fluorescent ligands in the exploitation of Orphan GPCRs for novel drugs

MSc Nanoscience Graduates 2011

Name	Dissertation Title
Ahmed Essam Alhadhrami	Synthesis and characterisation of Au, Ag and Cu nanoparticles and alloys
Razan Abdullah N Alshgari	Synthesis and characterisation of A Novel BODIPY-Dimer compound
Mehrnaz Behray	The Synthesis of lead sulphide quantum dots for in vivo imaging and apoferritin encapsulation
Elena Chesnokova	Protein encapsulation through a novel spray dried formulation
Madiha Fathi Elmahaishi	The role of substrate constraint in the cracking process
Nabila Mustafa Elhadi Elmrabet	Characterisation of Silicon-substituted Hydroxyapatite Thin Film Coatings on Titanium



PhD graduates

Our programme of training and development of Post Graduate students enhances their research and generic/ transferable skills base, and we provide a vibrant research environment (including the staging of national and international meetings). Participation at national and international conferences is at a very high level, with students winning competitive travel prizes from the Graduate School, travel bursaries from conference organisers, as well as industrial sponsorship and poster prizes at conferences. Travel Scholarships have enabled students to undertake placements in companies in South Africa, Japan, India, USA and China to develop greater awareness of the commercial and social relevance of their research.

PhD student	Thesis title	Supervisor
Dr Nurul Alam	Synthesis, characterisation and applications of meso/microporous silicate and carbon templated materials	Prof Robert Mokaya
Dr Martta Asikainen	Synthesis and gold-catalyzed transformations of allenic compounds	Prof Simon Woodward
Dr Frans Asmuruf	Quantum chemical calculations of the spectroscopy of core electrons	Dr Nicholas Besley
Dr Ian Barker	Innovations in mass transfer, biodegradable composites and hyperbranched polymer	Dr Derek Irvine
Dr Alexandre Bettoschi	Functionalised porous metal-organic frameworks for gas storage	Prof Martin Schröder
Dr Nicholas Butt	A Diels-Alder approach towards the pyrroindomycins	Prof Christopher Moody
Dr U. Butt	Investigation into conformationally-locked biaryazepine derivatives as catalysts for asymmetric synthesis	Prof Barry Lygo
Dr R. A. Castledine	A novel 1,3-dipolar cycloaddition strategy towards securinine and virosecurinine	Dr James Dowden
Dr Sarentha Chetty	Structure-based drug design of new inhibitors targeting InhA	Prof Neil Thomas
Dr Hainam Do	Molecular simulations of simple fluids	Prof Jonathan Hirst
Dr Marine Dufour	Indolequinones with anticancer activity	Prof Christopher Moody
Dr Benjamin Eade	Recycling and transport of chlorometallate complexes	Prof Martin Schröder
Dr Mark Franks	Transition metal complexes containing phenylthiolate and phenolate ligands	Dr Jonathan McMaster
Dr Fabio Ghiotto	The synthesis of functional analogues of the active site of [NiFe] hydrogenase	Prof. Martin Schröder Dr Jonathan McMaster
Dr J.A.R. Gilks	Development of catalysts derived from chiral amines	Prof Barry Lygo
Dr Alistair Green	Photoelectron spectroscopy as a probe of intramolecular vibrational dynamics in electronically excited toluene	Prof Katharine Reid
Dr Papia Haques	Continuous Clean Etherification	Dr Derek Irvine
Dr Mark Honey	A carbenoid approach to functionalized heterocycles	Prof Christopher Moody
Dr Bitu Birru Hurisso	UHV Spectroscopic Studies of Amino Acid-Based Ionic Liquids	Dr Pete Licence
Dr Lee Johnson	Synthesis of nanostructured metals using nanocrystals of cellulose	Dr Darren Walsh
Dr Daniel Lee	Development of high-resolution two-dimensional correlation spectroscopy in solid-state NMR	Dr Jeremy Titman
Dr Catherine Lucas	Synthesis of prenylated natural products utilizing pericyclic processes	Prof Christopher Moody
Dr Charlotte Mancel	Bio-inspired models of the active site of the (NiFe) hydrogenase	Dr Jonathan McMaster
Dr Dorothée Mancel	Complexes of [60]Fullerene	Dr Andrei Khlobystov Prof. Martin Schröder
Dr Andrew Parrott	Oligomeric PLA coupling agents for phosphate glass fibre/PLA composites	Dr Derek Irvine
Dr Katharine Portman	Structural studies of odorant binding proteins	Prof Mark Searle
Dr Diane Robbins	Two-directional methods for diversity and target oriented synthesis	Dr Rob Stockman
Dr C. Scotney	Investigations using chiral scandium(III) Lewis acids	Prof Barry Lygo
Dr Shalu Sharma	Structural and inhibitor investigations on Mycobacterial tuberculosis enzymes	Prof Neil Thomas
Dr Men Shuang	X-ray photoelectron spectroscopy of ionic liquid-based catalytic systems	Dr Pete Licence
Jill Sollenberger (MRes)	Biophysical studies of the molecular interactions of autophagy marker LC3B	Prof Mark Searle
Dr Mick Staniforth	Study of resonances in the ionization continuum of polyatomic molecules using photoelectron velocity map imaging	Prof Katharine Reid
Dr Emma Stephen	Redox non-innocence in transition metal macrocyclic complexes	Prof. Martin Schröder Dr Jonathan McMaster
Dr Haydn Williams	Computer simulations of protein folding	Prof Jonathan Hirst
Dr Carolyn Withers	Spectroscopic study of metal-rare gas complexes and the vibrational dynamics of para-fluorotoluene	Prof Timothy Wright
Dr Yu Wang	Fullerene (C_{60}) based metal-organic coordination polymers	Dr Andrei Khlobystov Prof Martin Schröder
Dr Yanqi Wu	New methods for measuring CSA tensors: applications to nucleotides and nucleosides	Dr Jeremy Titman
Dr Yong Yan	Metal-organic polyhedral framework materials for hydrogen storage	Prof Martin Schröder
Dr Sihai Yang	Modulating porosity in metal-oragnic frameworks	Prof Martin Schröder

GRADUATES

Research awards

Staff have been highly successful in competing for external research funds from a wide range of sources. Major awards have been obtained from the majority of the Research Councils (EPSRC, BBSRC, STFC, MRC and NERC) (70% of income), Charities (10%), the EU (10%) and Industry (10%). The largest sponsor is the EPSRC with funds awarded from the Chemistry, Materials, Life Sciences and Engineering Programmes.

Major new initiatives in metal-organic frameworks for hydrogen capture, extraction and catalysis have seen substantial awards in the form of an ERC Advanced Grant (£2.2M; 2008) and an EPSRC Programme Grant (£4.1M; 2011) which make Chemistry a key player in the University's wider energy agenda. A DTC in Hydrogen and Fuel Cells (with Birmingham and Loughborough) funds collaborative energy research with engineering.

RESEARCH AWARDS

Research Grants (Research Councils and Charities) Awarded 2011

Project Title	Investigators	Sponsor	Total
The Periodic Table of Videos: MolVids	Martyn Poliakoff Peter Licence Steve Liddle Debbie Kays Sam Tang Pete Licence	EPSRC	£325,249
Spectroscopy and Electron Transfer	Nick Besley	EPSRC	£430,777
New recyclable dioxyphosphorane polymers	Ross Denton	Royal Society	£14,830
Gas Adsorption at Structured Ionic Liquid Surfaces	Rob Jones Pete Licence	EPSRC	£552,179
Dimeric Diazoparaquinones Biosynthetic Speculation	John Moses	EPSRC	£341,506
Molecular and functional characterisation	Neil Oldham	BBSRC	£64,846
Combining Cryo-DNP and Rapid Temperature	Jon McMaster	EPSRC	£264,406
Design and Investigation of Near IR Dyes	Libby Gibson	Royal Society	£11,226
ChemEnSus	Martin Schröder Neil Champness Elena Bichoutskaia	EPSRC	£3,310,449
Modulated metal-organic frameworks	Martin Schröder Neil Champness	EPSRC	£427,297
Ensemble density functional methods for near-degenerate and excited states	Andrew Teale	Royal Society	£432,758
Development of a General sp2-sp3 Coupling Methodol	Rob Stockman	EPSRC	£141,892
Sustainable Phosphorus Chemistry: Catalytic Asymmetric SN2 Reactions	Ross Denton Neil Oldham	EPSRC	£344,114
Structural role of a unique p62 UBA dimer in the regulation of signal transduction and autophagy	Mark Searle	BBSRC	£261,899
Biomass Selective Valorization to Useful Feedstocks Under aqueous Conditions: Involvement in COST Action CM0903	Simon Woodward	EPSRC	£24,264
Wolsfon Research Merit Awards - Self Assembly of Photoactive Metal Organic Frameworks	Neil Champness	Royal Society	£90,000
Dorothy Hodgkin Fellowship - Nano-Magnets in Carbon Nanostuctures	Maria Del Gimenez-Lopez	Royal Society	£469,221
Complex Nanostructures by Supercritical Fluid Electrodeposition - Southampton lead	Mike George	EPSRC	£42,049
Acessing unusual f-Block oxidation states by electrochemistry	Steve Liddle	Royal Society	£12,737
Dynamic Structural Science at Research Complex at Harwell	Mike George	EPSRC	£388,143
UoN Promoting Sharing of Research Equipment	Mike George	EPSRC	£90,161
Synthesis of Amides from Nitriles via Multifaceted Catalysis	Jason Camp	EPSRC	£99,711
Jian Lu Royal Society SBFT Incoming Fellowship	Martin Schröder	Royal Society	£66,000
Oxidative processes - from amino acids to heterocycles, complexity from simplicity	Chris Moody	EPSRC	£341,242
The role of membrane rafts in cellular signalling	David Robinson	Leverhulme Trust	£61,813
Study of Bacillus subtilis DNA	Panos Soultanas	Wellcome Trust	£187,674
Biomimetic Asymmetric Synthesis	John Moses	Leverhulme Trust	£155,104
Leverhulme ECF - Selective gas capture, storage and conversion in functional prous hosts	Sihai Yang	Leverhulme Trust	£72,164
FTIR	Mike George	Leverhulme Trust	£29,738
FP7 - ERC - From Nano Test Tube to Nano Reactor: Visualisation Manipulation and Synthesis of Molecules at Nanoscale	Andrei Khlobystov	European Research Council	£1,254,757

RESEARCH AWARDS

Strategic Advisory Board

The School has established a strategic advisory board, involving captains of industry, high profile academics and government advisors to guide us with our strategy and to help maximise the impact of our research. Current membership includes:

Barry Stickings CBE, Chairman, had a distinguished 33-year career at BASF, retiring at the end of 2004. He remains active in the Chemical Industries Association (Council Member since 1993, Chair Responsible Care Board 1995-1999, President 1999-2001), was Deputy Chairman of the Chemicals Innovation and Growth Team set up by the UK Government in 2002 and Chairman of the UK Chemistry Leadership Council 2003-2006. He also chairs the board of Promethean Particles Ltd., one of the spin-out companies from the School.

Dr Glenn Crocker is Chief Executive of BioCity Nottingham, one of Europe's largest biotechnology incubators. He is also cofounder and director of R5 Pharmaceuticals ltd, a contract pharmaceutical formulation and manufacturing business, and is a director of Medilink East Midlands and Board adviser to Precos and Corinthian Surgical Ltd.

Steve Elliott is Chief Executive of the Chemical Industries Association. He is also Chair of AFEM (the European chemical trade association network), sits on the European Chemical Industry Council (Cefic)'s Board and Programme Council for Industrial Policy, Chair of the UK Energy Intensive User's Group and Vice-Chair of CBI's Trade Association Council.

Mark Gibson is currently the Chief Executive of The Whitehall & Industry Group, an independent, neutral, not-for-profit organisation which promotes co-operation and understanding between business and government. He was formerly the Director General of Enterprise and Business for the Department of Trade and Industry.

Dr Keith Layden is Chief Technology Officer and board member of Croda International PLC. He has held a number of Managing Director roles across Croda's European business. He is also a member of the Innovation Strategy Board for Chemistry Innovation and the Industrial Biotechnology Leadership Forum.

Professor W. Graham Richards, CBE was Head of Chemistry (1997-2006) at the University of Oxford. He is a Fellow of Brasenose College, Oxford and the author of 300 scientific articles and 15 books. He is a council member of the Royal Society of Chemistry and of The Royal Institution. He was a founder of Oxford Molecular Group Plc and Inhibox Ltd and is senior non-executive director of IP Group Plc.

Dave Allen joined GSK as a research chemist in 1981 and since that time has worked in a number of therapy areas, including antibiotics and cardiovascular medicines. He is now GSK's global chief chemist, head of respiratory medicine and is chair of the R&D Chemistry Council. In addition, he is the company's senior site leader for the Stevenage R&D site.

Ged O'Shea has been leading the research and development program for Alliance Boots Beauty brands for the past 4 years and is part of the leadership team that is driving strong business performance through product innovation. In addition, he leads the Boots Centre for Innovation that has pioneered Open Innovation and has delivered a global first to market in IPL technology for skincare.

David Brown has been IChemE's Chief Executive since late 2006. He spent 10 years at ICI in chemicals, polymers and biotechnology businesses and then ran a business unit for the University of Warwick before joining the consultants Arthur D Little Ltd in 1997 where, as Head of the Innovation, Research and Technology Practice, he was responsible for an extensive programme of work on innovation, research and technology exploitation at international, national, regional and company level, and on sustainable development.

Prof Paul Anastas is the Teresa and H. John Heinz III Professor in the Practice of Chemistry for the Environment at Yale. He is the Professor in the Practice of Green Chemistry with appointments in the School of Forestry and Environmental Studies, Department of Chemistry, and Department of Chemical Engineering. In addition, Dr. Anastas serves as the Director of the Center for Green Chemistry and Green Engineering at Yale. He was appointed by President Barack Obama to serve as the Science Advisor and Assistant Administrator for Research and Development for the US EPA.

Publications

Aireya, G. D., Wilmot, J., Grenfell, J. R. A., Irvine, D.J., Barker, I. A., and El Harf, J.i. (2011) Rheology of polyacrylate binders produced via catalytic chain transfer polymerization as an alternative to bitumen in road pavement materials. European Polymer J. 47, 1300-1314

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Alam, N., and Mokaya, R. (2011) Super-micropore/small mesopore composite pillared silicate and aluminosilicate materials from crystalline layered silicate Na-RUB-18. Microporous and Mesoporous Mater. 143, 104–114

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Baker, J. A., and Hirst, J. D. (2011) Molecular dynamics simulations using graphical processing units. Mol. Inf. 30, 498-504

Bartlett, P. N., Cook, D.C., George, M. W., Ke, J., Levason, W., Reid, G., Su, W., Zhang, W. J. (2011) Phase Behaviour and Conductivity Study of Electrolytes in Supercritical Hydrofluorocarbons. Phys. Chem. Chem. Phys. 13, 190-198

Bartrum, H. E., Blakemore, D. C., Moody, C. J., Hayes, C. J. (2011) Rapid Access to a-Alkoxy and a-Amino Acid Derivatives via Safe Continuous-flow Generation of Diazoesters. Chem. Eur. J. 17, 9586-9589

Batool, M., Martin, T. A., Abu Naser, M., George, M. W., Macgregor, S.A., Mahon, M. F., and Whittlesey, M. K. (2011) Comparison of the Photochemistry of Organometallic N-heterocyclic Carbene and Phosphine Complexes of Manganese. Chem. Commun. 11225-11227

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