**Introduction**
This booklet provides information about the research of individual members of academic staff within the Department of Chemistry. Web links have also been provided to allow you to access further information.

**Graduate Courses**

**Research Degrees in Chemistry:** The Department welcomes applications from excellent candidates to carry out research leading to the award of PhD and MSc degrees. MSc courses are 1 year in duration whilst PhD degrees are of between 3-4 years duration depending on the source of funding.

**Taught Masters: AS:MIT:** AS:MIT is delivered by internationally leading experts from the departments of Chemistry, Physics, Statistics, Engineering and the Life Sciences at Warwick, as well as visiting lecturers from companies such as Syngenta and Astra-Zeneca. Students gain hands-on practical experience with a wide range of equipment relevant to each module, enabling graduates from the course to work in any modern laboratory since the skills they will acquire are readily transferable between sub-disciplines.

**Interdisciplinary PhDs:** Warwick Chemistry participates actively in the MOAC (Molecular Organisation and Assembly in Cells) and Doctoral Training Centres. MOAC is home to a community of world-leading multidisciplinary researchers. Our training programme offers several courses at PhD and MSc level and focuses on developing the research leaders of tomorrow.

Our students have a range of diverse scientific backgrounds. We aim to provide more than just a traditional qualification, by equipping our students with the cross-disciplinary communication and transferable skills necessary to be successful in the competitive 21st century employment market. MOAC’s scientific focus is on developing and applying biophysical and theoretical tools to understand complicated molecular assemblies and machines in biological systems. The projects currently being done by our students can be found on their web pages.

**Research**
Warwick has an excellent international reputation for research and education in chemistry. Our staff win many national and international awards for science and innovation. We are firmly ranked among the top research departments in the UK (RAE2008). The Chemistry Department boasts some of the best laboratories and instrumentation in the UK with continuous heavy investment and expansion in equipment, facilities and people. We typically take on 50-60 new MSc and PhD students each year across our graduate programmes.

**Funding and Applications**

**Funding:** The department is very well supported by both Research Council and Industrial funding and we offer challenging projects across all aspects of modern Chemistry.

For further information please visit [http://www2.warwick.ac.uk/study/postgraduate/funding](http://www2.warwick.ac.uk/study/postgraduate/funding)

**Applications:** You have to apply using the online application system please visit:
[http://www2.warwick.ac.uk/study/postgraduate/funding](http://www2.warwick.ac.uk/study/postgraduate/funding)
Research Summary
We study the Inorganic Biochemistry of metal-binding proteins from a variety of organisms including mammals, invertebrates, plants, and bacteria, with the aim to contribute to the understanding of mechanisms of metal ion homeostasis. Protein structure, dynamics of metal uptake and release, and biomolecular interactions are studied using recombinant protein expression and purification, multinuclear NMR, mass spectrometry, optical spectroscopies and multi-elemental analysis.

Biological Inorganic Chemistry
All organisms require essential metal ions (e.g. Ca, Co, Cu, Fe, and Zn) for survival, but excesses of the same metal ions are harmful, and can lead to disease and death. Therefore, all life forms have developed intricate mechanisms to regulate the levels of these metal ions, and to ensure that they are delivered to the 30-50% of metallo-proteins that make up any given proteome.

Many new proteins involved in metal transport have been identified in recent years, yet very little structural information is available, limiting our understanding of mechanisms. Important questions remain about how a protein acquires the correct metal, and how toxic elements such as cadmium are dealt with. Our research aims to elucidate principles that govern metal selectivity of proteins involved in zinc and copper ion transport, using 3D structure determinations accompanied by thermodynamic and kinetic studies.

Selected Publications


Further Information
http://www2.warwick.ac.uk/fac/sci/chemistry/research/chemicalbiology/blindauer/blindauergroup

c.blindauer@warwick.ac.uk

+44 (0) 2476 528264
Research Summary
Supracolloidal polymer chemistry. Design of supracolloidal structures through liquid-liquid interface driven assembly of colloidal building blocks. Particle stabilized heterogeneous polymerization strategies are used to fabricate a variety of structures: raspberry structured hybrid nano- and microcapsules, biomimetic inorganic skeletons via multistage assembly routes, non-spherical liquid droplets, multifaced patchy particles.

Research Statement
We study the chemistry and physics of colloidal systems in which molecular and/or colloidal entities can be assembled into more complex supracolloidal structures. We are interested in the synthesis of particles and macromolecules with a design tailored to trigger and control motility and assembly, the development of methods to (self-)organise colloidal matter, the understanding of the interactions involved between molecular and colloidal building blocks and potential macroscopic substrates. We find it important that our technology can be scaled-up and is of use in a variety of industrial applications ranging from sensors and devices, coatings and adhesives, to food, personal care, agricultural and biological systems.

Selected Publications

Further Information
http://www2.warwick.ac.uk/fac/sci/chemistry/research/materialschemistry/bon/bongroup
s.bon@warwick.ac.uk
+44 (0) 2476 574009
Prof. Timothy D. H. Bugg
MA (Cantab), PhD (Cantab), CChem MRSC
Professor of Biological Chemistry

Research Summary
Understanding of important enzyme-catalysed reactions, using a combination of the following techniques: synthesis of enzymatic substrates and inhibitors, isotope labelling experiments, enzyme purification and enzyme kinetics. Major areas of interest are enzymes involved in the bacterial degradation of aromatic compounds, and enzymes involved in bacterial cell wall peptidoglycan biosynthesis, as targets for the development of novel antibacterial agents.

Research
Research in my group is in the areas of biological chemistry and mechanistic enzymology. Enzymes are biological catalysts which speed up all of the biochemical reactions found in Nature. They are wonderful catalysts whose speed of catalysis, selectivity and specificity far exceed man-made catalysts, they are capable of catalysing reactions which have little or no precedent in Chemistry, and they do all of this in water at pH 7, room temperature! Enzymes have many important applications in biotechnology, and there are many enzyme-catalysed reactions which represent good targets for therapeutic action via selective enzyme inhibition.

The two major areas of interest are: enzymes involved in the bacterial degradation of aromatic compounds in the biosphere; and enzymes involved in the assembly of bacterial cell wall peptidoglycan.

Selected Publications


Further Information
http://www2.warwick.ac.uk/fac/sci/chemistry/research/chemicalbiology/bugg/bugggroup
l.d.bugg@warwick.ac.uk
+44 (0) 2476 573018
**Research Summary**
Natural products chemistry and biology, including isolation and structure determination of new bioactive natural products, genomics and genetics of natural product biosynthesis, enzymology of natural product biosynthesis, chemical synthesis of bioactive natural products and intermediates in their biosynthesis, genetic manipulation of bioactive natural product biosynthetic pathways to produce new analogues, molecular mechanism of action of bioactive natural products and their biological function. A highly multidisciplinary approach to these problems is taken encompassing high field NMR spectroscopy, mass spectrometry, organic synthesis, bioinformatics, microbiological methods, molecular genetic manipulation, recombinant protein overproduction, purification and biochemical/biophysical characterisation.

**Current Research Projects**
Natural products are both beneficial and detrimental to human existence. On the plus side, natural products continue to enjoy wide spread human application as life-saving medicines and environmentally benign agrochemicals that enhance the quality of our daily lives. Their production by extraction from biomass is fully compatible with the current drive towards a sustainable low-carbon economy based on plant feedstocks rather than petrochemicals. However, many natural products are toxins that are harmful to humans, or virulence factors that help pathogenic microbes to infect their hosts. Natural products also play an important role in cellular signalling in a variety of organisms.

Understanding the molecular mechanisms by which natural products are biosynthesised and interact with biological systems are key themes that underpin much of my group’s research. Such understanding can be exploited in several different ways. For example, it can be used to guide the discovery of novel bioactive natural products by mining the genome sequences of microbes and plants; it can be applied to the bioengineering of biosynthetic pathways responsible for the assembly of potentially useful metabolites to produce structurally novel derivatives with superior properties; and it can form the basis for designing inhibitors of enzymes on pathways for the assembly of detrimental natural products, like virulence factors and toxins.

We are actively engaged in elucidating the biosynthetic pathways to numerous bioactive natural products including antibacterials, antimalarials (e.g. streptorubin B), antivirals, anticancer agents, phytotoxins, mycotoxins, virulence-conferring siderophores and signalling molecules. We also have a vibrant programme of novel bioactive natural product discovery that employs state-of-the art genomics based approaches alongside more traditional screening approaches and we recently completed the first total synthesis of a natural product discovered by the group. We are exploring the potential of bioengineering for the production of novel natural product analogues and are dissecting the molecular mechanisms for recognition of several natural products by their biological targets.

A lively and vibrant spirit that embraces the challenges of cutting edge research at the interface of chemistry and biology pervades the group, which is housed in top quality, recently refurbished laboratories, equipped with some of the best facilities for research at this interface in the world. This environment provides scientists at the masters, Ph.D. and postdoctoral levels with unequalled research training in Chemical Biology.

**Selected Publications**


**Further Information**
http://www2.warwick.ac.uk/fac/sci/chemistry/research/chemicalbiology/challis/
g.l.challis@warwick.ac.uk
+44 (0) 2476 574024
Dr. Andrew J. Clark  
BSc, PhD (London)  
Associate Professor of Organic Chemistry

**Research Summary**
Free radical chemistry in organic synthesis. Development of atom transfer radical cyclisations, radical-polar crossover reactions and cascade processes in natural product synthesis. Chemical biology, phage display and plant biochemistry. Use of plant oils to manufacture polyurethanes, epoxy resins and phenolic polymer composites, chemistry of cellulose, hemicellulose and lignin.

**Research**
Our recent research covers these main areas of synthetic chemistry:
- The development of new methodology and application to natural product synthesis using free radicals (including chemistry of enamides and ynamides).
- The development of renewable resources as feedstocks for the chemical and polymer industries (including processing of waste products to valued added materials).
- The application of chemical genetics tools to help in determining drug/receptor interactions

In collaboration with the Warwick Manufacturing Group and WarwickHRI we prepared materials from vegetable oils that were used in plastics found on the eco-car. The eco-car has appeared at the Eden Project, the Science Museum in Kensington, the Top Gear website and will soon be an exhibit at the Coventry Motor Museum.

Recently, we prepared the fuel for the F3 World First Racing car. We recently were awarded two grants to continue work in the area of renewables. Adaptive Processing of Natural Feedstocks: EPSRC EP/F015321/1 (£475,878). Wealth out of Waste: Warwick Innovative Manufacturing Research Centre (£2,324,000). We are working closely with Boots, Croda, Akzo Nobel and Ci-KTN to exploit this research.

**Atom Transfer Radical Cyclisation**
Transition metal catalysed atom transfer radical cyclisation (ATRC) and polymerisation (ATRP) reactions have been extensively studied over the last few years. The driving force for this research has been the desire to find non-reductive catalytic alternatives to organotin hydrides in mediating radical cyclisation reactions in organic synthesis, and the need to prepare living polymers with a high degree of control for novel materials applications. We have introduced a range of new ligands for these processes (see Fig. 1).

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**Selected Publications**


Copper(I) mediated tandem 1,4-arylation migration / oxidative 5-exo amidyl radical cyclisation of bromosulfonylamides, A. J. Clark, D. R. Fullaway, N.P. Murphy, H. Parekh, Synlett, 2010, 610.


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**Our Research interests span many areas...**

- Synthetic methodology and Natural Products
  - Atom Transfer Radical Cyclisation Reactions
  - Synthetic Methodology using Radicals
  - Synthetic Methodology using Hydroxamic acids
  - Synthetic Methodology using Zirconium

- Materials and Green Chemistry
  - Materials from Renewable Resources
  - Dendrimers
  - Atom Transfer Polymisation
  - Adaptive Processing of Natural Feedstocks (awaiting IP agreement before releasing information)
  - Evolvable Process Design (awaiting IP agreement before releasing information)
  - Wealth out of Waste (awaiting IP agreement before releasing information)
  - Electrospinning

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**Further Information**
http://www2.warwick.ac.uk/fac/sci/chemistry/research/syntheticchemistry/clark/  
a.j.clark@warwick.ac.uk  
+44 (0) 2476 523242
Research Summary
Improving the performance and applications of Fourier Transform Ion Cyclotron Resonance (FTICR) mass spectrometers. We work collaboratively with other research groups to demonstrate the effectiveness of higher specification FTICR mass spectrometry in specific applications. Particular focus in recent years has been on fundamental studies of the mechanism of electron capture dissociation, FTICR instrument design, post-translational modification analysis of proteins and peptides, deamidation and isomerization of aspartic acid residues in peptides and proteins, etc.

Peter O’Connor Group
Mission:
1. To develop new FTICR mass spectrometry instruments with unique capabilities.
2. To apply these FTICR mass spectrometers to interesting and difficult questions in chemistry, biochemistry, and medicine.
3. To teach students and postdocs about these tools and their uses.

History:
Peter O’Connor moved to the Warwick Chemistry department, starting January 1, 2009. Before this he developed a FTICR based instrumentation group at Boston University (www.bumc.bu.edu/FTMS). The plan is to build a similar, but bigger centre for FTICR mass spectrometry here at Warwick, over the next decade or so.

Instruments:
1. A Bruker 12T Solarix FTICR mass spectrometer with ESI, nESI, MALDI, APPI, LCMS, GCMS, and APCI capabilities along with ECD and IRMPD.
2. This instrument is currently being built. It is planned as a 12 T ESI FTICR with added features. See here.
3. A 4.7T AS Electrospray FTICR mass spectrometer generously donated by Ernest Laue of Cambridge University.

Selected Publications


Further Information
http://www2.warwick.ac.uk/fac/sci/chemistry/research/physicalchemistry/oconnor/
p.oconnor@warwick.ac.uk
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Research Summary

New chemical keys to unlock the production of novel microbial antibiotics. Understanding the details of the regulation of antibiotic biosynthesis in actinomycete bacteria, from which more than 70% of clinically-approved antibiotics originate. Exploiting signalling molecules (microbial hormones) to induce production of novel antibiotics in the laboratory environment.

Research Interests

Over the last 25 years, the discovery of novel antibiotics has declined dramatically, and, in the past 2 years only 1 antibacterial agent was approved for clinical use in the US.[1] This would not be so alarming if the incidence of drug-resistant bacterial strains had stagnated, but these “Superbugs” have been proliferating rapidly.[1] With the antibiotic pipeline running dry, and with the pharmaceutical industries reluctance to invest in anti-infective discovery, novel strategies urgently need to be developed and applied to drug discovery. Since the discovery of penicillin in 1928, the main source of antibiotics has been micro-organisms. More than 70% of commercially available antibiotics are produced by Streptomyces bacteria.[2] Following the sequencing of the entire genome of Streptomyces coelicolor A3(2), which is widely accepted as the model actinomycete, an unexpectedly large number of antibiotic-like gene clusters were found to be encoded within Streptomyces genomes.[3] Many of these so-called cryptic gene clusters (cryptic because their products are not known) were predicted to encode for the biosynthesis of novel bioactive natural products. Such genome mining has resulted in the development of new strategies for isolating and characterising the metabolite products of these previously unknown gene clusters.[4]

Under laboratory culture conditions, these cryptic biosynthetic gene clusters are often not expressed. Consequently, new approaches are needed to access this untapped biosynthetic potential. The production of several Streptomyces secondary metabolites is triggered by gamma-butyrolactone (GBL) inducer molecules, the most characterised of which is A-factor (Fig. 1) made by Streptomyces griseus.[5] In the model streptomycete S. coelicolor A3(2), GBLs (S. coelicolor butyrolactones or SCBs, Fig. 1) directly regulate the production of a polyketide antibiotic of unknown structure.[6]

A-factor (GBL)

SCB1 (GBL)

MMF1 (AHFCA)

Fig. 1 Structures of molecules that specifically induce antibiotic production in Streptomyces bacteria

Through a genome mining approach, we have recently discovered a novel structural class of inducer molecules [2-alkyl-4-hydroxymethylfuran-3-carboxylic acids or AHFCAs, exemplified by MMF1, Fig. 1] made by S. coelicolor A3(2).[7] MMF1 specifically induces the production of methylenomycin A, one of the several antibiotics known to be made by this bacterium. Comparative genomics and a literature survey have shown the likely prevalence of AHFCAs in other bacteria.

Selected Publications


Further Information

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+ (44) 2476 150 170
Research

Our research is focussed on the spontaneous organisation of molecular building blocks into nanostructures having novel electronic, optical, magnetic and catalytic properties.

A key issue in nanotechnology is the development of conceptually simple construction techniques for the mass fabrication of nanoscale structures reaching down to the atomic scale. At this level conventional top-down fabrication paradigms become unusable. The natural alternative is self-organized growth, where nanoscale arrangements are built from their atomic and molecular constituents by processes intrinsically providing structural organization.

In particular, supramolecular self-assembly is a very attractive strategy to achieve this goal both for its efficiency as well as for the high structural quality that can be obtained.

Selected Publications


Further Information

http://www2.warwick.ac.uk/fac/sci/chemistry/research/physicalchemistry/costantini/
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Research Summary
Design and implementation of new computer modelling methods for molecular transition metal systems: Code development for transition state searching, Jahn-Teller distortions, and spin-state effects such as thermal spin crossover (SCO) and light-induced excited spin state trapping (LIESST). Applications in co-ordination, organometallic and bioinorganic chemistry with special emphasis on Cu(II), Fe(II), Pt(II) and Ru(II) in simple complexes, anti-cancer agents and metalloenzymes.

Research
Development and application of computational methods to systems containing transition metal centres
While DFT is often the method of choice for quantum chemical treatments of TM systems, all quantum approaches are slow. QM can never hope to treat completely really large systems like, for example, proteins. In contrast, empirical schemes based on classical mechanics are efficient enough for such large systems but TMs present significant problems. The d electrons are stereochemically and energetically 'non-innocent' and must be included - explicitly or implicitly - in the computational model. Conventional Molecular Mechanics can only deal with a limited range of these d-electron effects. It struggles, for example, with Jahn-Teller effects and other geometrical distortions - spin state changes - arising from the 'stereochemical activity' of an incomplete shell of d electrons such. Consequently, we are developing a unique MM scheme which extends conventional MM by adding a d-electron energy term derived from generalised Ligand Field Theory. This Ligand Field Molecular Mechanics (LFMM) model has been applied to the Jahn-Teller distortions of Cu(I) complexes and a variety of other copper systems, including Type I 'blue' proteins; manganese(II) carboxylate complexes, including bimetallic species; bimetallic copper complexes and more. We are constantly extending and enhancing the method both with respect to its basic functionality - e.g. ligand field molecular dynamics, automatic parameter optimisation - and with respect to wider ranges of TM complex. Parameter files are available elsewhere on the site. The method has been implemented in the Molecular Operating Environment developed by Chemical Computing Group, Montreal.

We also have a beta-test version of DL_POLY2 with our LFMM method included which we hope to release soon. The problem with DL_POLY is that it's designed for MD and its simple energy minimisation capabilities are pretty primitive.

Selected Publications


Further Information
http://www2.warwick.ac.uk/fac/sci/chemistry/research/computationalchemistry/deeth/
rj.deeth@warwick.ac.uk
+44 (0) 2476 523187
Dr. Ann M. Dixon
Associate Professor of Biological Chemistry

Research Summary
Developing methods for describing the assembly, interactions and three-dimensional structures of membrane proteins using biophysical and computational techniques, including NMR spectroscopy. Of particular interest are membrane proteins associated with virally-induced cancers, which have demonstrated membrane protein-mediated mechanisms of cellular transformation.

Membrane Protein Structure, Assembly and Folding Group
Membrane proteins comprise over a third of the human genome, and a significant fraction of other known genomes. Helical membrane proteins in particular are emerging as the principal drug targets for a wide variety of diseases.

Despite their obvious importance, very little structural information has been obtained on this class of proteins. This is chiefly due to difficulties in the production and purification of membrane proteins, and the requirement of lipids or detergents to solubilize these proteins.

However, our growing understanding of detergents and lipids and the development of new formulations to solubilize membrane proteins has moved the field forward significantly.

Selected Publications


Further Information
http://www2.warwick.ac.uk/fac/sci/chemistry/research/chemicalbiology/dixon
ann.dixon@warwick.ac.uk
+4 (0) 2476 150037
Dr. Andrew Dove
MChem (York), PhD (Imperial)
Associate Professor of Chemistry

Research Summary

Degradable Biomaterials and Sustainable Polymers
The development of novel degradable biomaterials is largely restricted by the paucity of well-defined functional degradable materials. As such, a major focus of our research is the synthesis of poly(ester)s by ring-opening polymerisation (ROP), poly(carbonate)s by both ROP and CO₂/epoxide copolymerisation as well as the synthesis of polymers with more diverse backbones including poly(phosphoester)s and poly(ortho ester). Our work leads us to examine a range of disciplines including the development of non-toxic catalysts, materials characterisation and supramolecular self-assembly focussed towards the discovery of novel hydrogel materials, photocrosslinked 3D tissue-engineering scaffolds by microstereolithography and active materials for delivery of therapeutic reagents.

As a consequence of the degradable nature of the polymers, unique and innovative strategies are required to achieve our goals. Furthermore, in the course of this work many of our starting materials can be preferentially derived from renewable and sustainable resources such as CO₂, sugars and amino acids. A particularly exciting aspect of this approach results from the chiral nature of many of the monomer precursors thus offering unique opportunities to control the materials properties and self-assembly simply by control and manipulation of the polymer stereochemistry.

Research Interests
- Polymerisation catalysis
- Synthesis of functional degradable polymers from sustainable resources
- Biohybrid polymers
- Self-assembly and ordering of degradable polymers
- Development of novel degradable biomaterials

Selected Publications
Synthesis and Organocatalytic Ring-Opening Polymerization of Cyclic Esters Derived from L-Malic Acid

Development of Amino-Oxazoline and Amino-Thiazoline Organic Catalysts for the Ring-Opening Polymerisation of Lactide

One-Pot Synthesis of alpha,omega-Chain End Functional, Stereoregular, Star-Shaped Poly(lactide)

Metal free thiol-maleimide ‘Click’ reaction as a mild functionalisation strategy for degradable polymers

Further Information
http://www2.warwick.ac.uk/fac/sci/chemistry/research/materialschemistry/dove/
a.p.dove@warwick.ac.uk
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Research Interests
1) Medicinal chemistry - drug discovery, such as clinical candidate FX125L for inflammatory diseases such as asthma and related conditions, and the development of mechanistic probes for the discovery of new biological mechanisms.

2) Reaction mechanism of asymmetric and catalytic processes using kinetics and DFT modelling - organolithium reactions, transition metal catalysed reactions and organocatalysis.

Organic Synthesis: Mechanism and Applications
We are interested in synthetic and mechanistic organic chemistry. Our research covers a range of subjects, generally in these areas:
- Synthetic drug discovery, the development of mechanistic probes for the discovery of new biological mechanisms and natural product synthesis. One of our anti-inflammatory drug candidates, FX125L, is in phase 2 clinical trials, and shows great potential as a treatment for inflammatory diseases.
- Mechanistic investigation and optimisation of asymmetric and catalytic reactions and DFT modelling - organolithium reactions, transition metal catalysed reactions and organo-catalysis.

Fox Group Research
Medicinal Chemistry - the synthesis of anti-inflammatory drugs, new peptide mimetics and the other interesting biologically active small molecules and peptides.

Asymmetric Catalysis Kinetics and Mechanism - new methods for analysing and optimising catalytic and asymmetric reaction systems.

Computational Organometallic Chemistry - stereoselective organolithium reaction, organo-transition-metal catalysis and organocatalysis.

Selected Publications


Further Information
http://www2.warwick.ac.uk/fac/sci/chemistry/research/syntheticchemistry/fox/
d.j.warwick.ac.uk
+44 (0) 2476 524331
Dr. Matthew I. Gibson
MChem (Hons), Ph.D (Dunelm), MRSC,
Science City Fellow

Research Summary
Design of membrane-interacting macromolecules to aid in cryopreservation, specific membrane disruption or to trigger cellular uptake. We are also developing environmentally responsive polymers and nanoparticles as well as [glyco]polymers for targeted delivery of therapeutics and to prevent/treat infection. The work is highly interdisciplinary crossing the boundaries of fundamental organic and polymer chemistry with the life sciences.

Research
All our research is inspired by biological systems. For example, inspired the by antifreeze glycoproteins (AFGPs) found in polar fish species, we are developing novel macromolecules which can reproduce their properties, and using these for the cryostorage of organs ultimately. Conversely, we are mimicking peptides found in every human, which act to destroy bacterial membranes. We are using these as novel antibiotics. We are also interested in stimuli-responsive polymers (see example below) for “trigger” polymers/nanoparticles to have a particular effect, such as self-assembly or drug release.

Stimuli Responsive Polymers and Nanoparticles
We showed that polymer-coated nanoparticles display size-dependent LCST behaviour, with larger particles have lower transition temperatures. Furthermore, mixtures of nanoparticles displayed cooperative aggregation indicating this as a simple method for fine tuning nanoparticle LCST with implications for drug-delivery systems. Finally, we exploited this to guide nanoparticle assembly onto complementary surfaces which could be used as a slow release depot or as a sensor platform.

Selected Publications


Further Information
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Prof. David Haddleton
BSc, DPhil York
Professor of Chemistry

Research Summary
New methods of polymer synthesis and catalysis. Specific interests include controlled polymerisation of acrylics and esters by organometallic initiators and catalysts, e.g. atom transfer living polymerisation, catalytic chain transfer polymerisation. Mechanisms of polymerisation and utilisation of this knowledge to design catalysts and organic polymers for specific commercial applications. Environmentally friendly polymerisation and use of biomimetic chemistry in this area.

About the Polymer Group
The central theme of our research is controlled polymerisation to give macromolecules of designed, desired and targeted structure. Work is directed to the synthesis of polymers one monomer at a time in an attempt to approach the degree of sophistication exhibited by natural polymers. An overriding aspect of all of our work is the desire to use environmentally friendly processes which are viable on the commercial scale.

Work is carried out to use existing polymerisation methodology to build polymers of specific geometry whilst attempting to understand the mechanisms of polymerisation. We currently have projects to synthesise block copolymers, star copolymers and dendrimers. We firmly believe that in order to fully utilise a polymerisation system we must fully understand the chemistry. This leads to our work being a hybrid between organometallic catalysis and traditional polymer synthesis.

We are also very interested in extending the scope of living polymerisation to monomers which fall outside the traditional areas of anionic and cationic polymerisation, namely a range of functional monomers and monomers with no electron withdrawing or donating substituent attached to the polymerisable double bond. Characterisation is by state-of-the-art methodology including MALDI-TOF-MS and LALLS GPC as well as extensive use of conventional GPC.

Selected Publications
Phosphine-mediated one-pot thiol-ene “click” approach to polymer-protein conjugates

Glycopolymers via catalytic chain transfer polymerisation (CCTP), Huisgens cycloaddition and thiol-ene double click reactions, L. Numi, J. Lindqvist, R. Randev, J. Syrett and D. M. Haddleton, Chemical Communications 2009, 19, 2727-2729


Further Information
http://www2.warwick.ac.uk/fac/sci/chemistry/research/materialschemistry/haddleton/
d.m.haddleton@warwick.ac.uk
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Research Summary
The development of nanostructured electrodes and light harvesting organic semiconductors for utility in organic solar cells. The primary aim is to increase the efficiency with which these thin film devices convert sunlight into electricity whilst retaining the cost advantage afforded by the use of organic semiconductors.

Selected Publications


Further Information
http://www2.warwick.ac.uk/fac/sci/chemistry/research/physicalchemistry/hatton/
ross.hatton@warwick.ac.uk
+44 (0) 2476 150874
Prof. Tim Jones

BSc (Liverpool), PhD (Liverpool)
Professor of Physical Chemistry

Research Summary

Controlling the growth and properties of a wide range of semiconductor thin films and nanostructures, using both inorganic and organic materials. A sophisticated array of thin film deposition techniques is used to develop new types of structures with novel and well-defined functional properties (i.e. electronic, optical or magnetic), and prototype devices are developed in areas such as solar cells, sensors and spintronics. Current research includes: Organic solar cells; Hybrid organic-inorganic solar cells; Molecular magnetism and spintronics; Molecular assembly at surfaces and control of interface properties; Growth of indium nitride alloys and nanostructures; III-V semiconductor nanostructures for high efficiency solar cells; Novel narrow band gap semiconductor materials for infrared sensing applications.

Research

The group's research is focused on controlling the growth and properties of a wide range of thin films, nanostructures and complex heterostructures, using both inorganic and organic semiconductor materials. The overall aim is to develop new types of structure with novel and well-defined functional properties (i.e. electronic, optical, magnetic or optoelectronic), and then to exploit them through the development of innovative device structures. Particular emphasis is placed on correlating thin film property with growth mechanism; the control of surface and interface properties; the development of multilayer structures and heterostructures with novel properties; and the fabrication and assessment of prototype device structures for applications in areas including solar cells, sensors and spintronics. We collaborate extensively with other research groups in Warwick (in Chemistry, Physics and Engineering), as well as with many groups at other UK and overseas universities and research institutes. We also have excellent links with several industrial companies.

Current research projects are focused in the following areas:

1. Molecular solar cells
2. Hybrid organic-inorganic solar cells
3. Molecular magnetism and spintronics
4. Molecular assembly and control of surface properties
5. Growth of indium nitride alloys and nanostructures
6. III-V semiconductor nanostructures for very high efficiency solar cells
7. Novel narrow gap semiconductor materials for chemical sensing applications

Selected Publications


Further Information

http://www2.warwick.ac.uk/fac/sci/chemistry/research/physicalchemistry/jones/jonesgroup

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+44 (0) 2476 528265
Prof. Julie Macpherson
BSc, PhD Warwick
Professor of Chemistry

Research Summary
Development of new scanned probe techniques for nanoscale imaging; development of new electrode materials based on carbon materials (conducting diamond and carbon nanotubes) for sensing applications, electrochemical and electronic device fabrication, and structural and chemical characterisation of surfaces. A range of techniques are employed, for example, atomic force microscopy (AFM), modified for electrical and electrochemical measurements; (ii) scanning electrochemical microscopy (SECM); (iii) SECM-AFM; (iv) electron microscopy; (v) microfabrication; (vi) Raman

Research
Our research focuses on the application of electrochemistry to the understanding of fundamental and practically important interfacial chemical processes at the micro to nanoscale.

A significant aspect of our work is the development and application of new techniques, which can provide a greater understanding of this wide area of science. Processes studied experimentally encompass the biomedical/life sciences and materials science, as well as chemistry. Supporting theoretical work involves the development of models for mass transport and coupled chemical reactions in heterogeneous systems.

The development of nanoscale methods is of particular interest and this has led to recent interest in the use of single walled carbon nanotubes for a variety of applications, including AFM probes, conducting probes and electronic device applications.

We are also interested in the application of novel conducting diamond hybrid materials for sensor applications.

Selected Publications


Further Information
http://www2.warwick.ac.uk/fac/sci/chemistry/research/physicalchemistry/macpherson/
j.macpherson@warwick.ac.uk
+ (0) 2476 573886
Dr. Andrew Marsh
B.Sc., Ph.D. (London), MRSC, CChem
Associate Professor of Chemistry

Research Summary
Combining organic chemistry and molecular design in the synthesis of functional molecules.
To understand how the molecules we make interact with each other and with biological targets we use a range of techniques including isothermal titration calorimetry, gel permeation chromatography and NMR. Discovery of protein targets for known bioactive molecules using phage display, and engineering bioinert surfaces are just two areas we have worked on in collaboration with other groups recently.

Selected Publications
Using the Man9(GlcNAc)2 – DC-SIGN pairing to probe specificity in photochemical immobilization


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Dr. Rebecca Notman

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Science City Research Fellow

Research Summary
Molecular simulations of biomolecules and materials systems, at both the atomistic and coarse-grained levels. Research includes simulations of peptides interacting with inorganic surfaces, biological membranes and the transport of molecules across membranes, and the molecular structure and organisation of the stratum corneum skin barrier. An additional area of interest is drug delivery and nanomedicine, including characterisation of advanced materials for biomedical applications and transdermal drug delivery.

Research
We use molecular dynamics computer simulations to explore the properties and functions of biological molecules and materials at the molecular level. Of particular interest are biological membranes, including the phospholipid membranes that surround our cells and the ceramide lipid layers that comprise the human skin barrier. We are also interested in peptides and proteins, including transmembrane helical peptides, structural intermediate filament proteins and protein-DNA interactions. Another aspect of research considers the interactions between biological molecules and inorganic materials. This is important for a range of applications in bionanotechnology. For example, one project aims to understand the uptake of nanoparticles into cells, which will help to address concerns of nanotoxicity and also assist in the design of multi-functional nanoparticles for biomedical applications.

Selected Publications


Further Information
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Dr. Rachel O’Reilly
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Research Summary
Design, synthesis and application of uniquely derived polymeric materials; where control over architecture, functionality and reactivity are central to their application in the field of nanotechnology. Interdisciplinary research bridging the interface between synthetic, polymer and catalysis chemistry, allowing for the development of materials that are of importance in medical, materials and nanoscience applications.

Research
Our research targets the design, synthesis and application of uniquely derived polymeric materials; where control over architecture, functionality and reactivity are central to their application in the field of nanotechnology. We are especially concerned with the synthesis of polymeric materials using both established chemistries and developing new synthetic polymerisation strategies. The supramolecular assembly of these polymers into precision nanostructures, such as organic/inorganic or hybrid nanoparticles is of interest given their ability to mimic biomolecules in size, structure and function and also possess novel properties, including the ability to behave as hosts or vessels in delivery agents.

The subsequent assembly of these nanoparticles in one-, two- and three dimensions, and their chemical modification, can be applied to afford materials with potential applications as biological mimics, nanoreactors and nanotechnology devices.

Our overall research is highly interdisciplinary and is orientated towards bridging the interface between creative synthetic, polymer and catalysis chemistry, to allow for the development of materials that are of significant importance in medical, materials and nanoscience applications. This involves the application of controlled polymerisation chemistries for the synthesis of macromolecular structures and their functionalisation and application using materials chemistry.

Selected Publications


Further Information
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Prof. Alison Rodger
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Professor of Biophysical Chemistry

Research Summary
Biomacromolecule structure and function especially DNA, membrane proteins and fibrous proteins; Intermolecular interactions; Developing new polarised spectroscopy techniques for biomacromolecules. Particular expertise in circular and linear dichroism, fluorescence. Analytical chemistry, especially as related to biological applications.

Biophysical Chemistry
We are a group working in bioanalytical and biophysical chemistry. Our main areas are spectroscopy, particularly ultra-violet spectroscopy including circular and linear dichroism. The samples we study include a wide range of proteins, their interactions with DNA and carbon nanotubes. We also develop instrumentation, particularly for linear dichroism.
Our backgrounds are diverse. Alongside chemistry, there are group members who have trained in mathematics, biology and physics departments, with a wide range of expertise and experience. We are always open to new ideas and collaborations to develop the techniques and instruments we work with.

Research Interests
Our current research interests include the following:
- Circular dichroism
- Linear dichroism
- Control of DNA structure by synthetic metallomolecules
- Carbon nanotubes
- Prokaryotic cell division proteins
- Membrane proteins
- Fibrous proteins
- Kinetics of restriction enzymes

Selected Publications

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Research Summary

Understanding and predicting the physical properties of liquids, solids and their interfaces. Current methodological developments focus on ways of simulating infrequent events directly with Molecular Dynamics. Applications include: design of low dosage additives to suppress crystallisation from oils and water; theory and properties of clathrate formation; metal-organic framework compounds; simulations of crystal nucleation and growth, including biomineralisation; and characterising drug / biomolecule interactions.

Molecular Simulations at Warwick

What we do...

We are a classical modelling group with several unique project areas, ranging from Asphaltenes, Wax and corrosion to Hydrates, Bio-molecules through to Materials. We concentrate on thermodynamic and structural properties as well as intense studies of growth mechanism. Inhibition of crystal growth is studied with the cesium formate and former wax inhibitors. While growth is encouraged in hydrate structure of both methane and carbon dioxide.

Selected Publications


Further Information

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Dr. Jon Rourke
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Associate Professor of Chemistry

**Research Summary**
Mechanistic studies of organo-palladium and platinum species are being undertaken with a view to understanding C-H activation processes. In addition, organometallic liquid crystals based on platinum and palladium. Inorganic and organometallic ‘molecular materials’ are being developed which utilise the fundamental properties of their constituent molecules rather than bulk properties of the sample. These are being used as bases of new varieties of liquid crystal and functionalised sol-gel glasses.

**Research**
Jon Rourke’s research group is interested in a wide variety of organometallic chemistry. In particular we are currently interested in mechanistic aspects of the C-H activation reaction and the coordination of unusual ligands. Details from recent projects are described briefly below (more information is available from the papers we have published).

**Organo-platinum chemistry**
Currently, our primary focus is on the organometallic chemistry of platinum, and we have a number of active projects in this area.

A recent highlight has been the identification of an agostic complex that shows a delicate balance between the activation of sp² and sp³ hybridised C-H bonds.

**Selected Publications**


**Further Information**
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Research Summary
Chemistry of metals in medicine (bioinorganic chemistry, inorganic chemical biology and medicine). Design and chemical mechanism of action of therapeutic metal complexes, including organometallic arene anticancer complexes, photoactivated metal anticancer complexes (for photochemotherapy), metallomacrocycles as antivirals and stem-cell-mobilising agents, and metalloantibiotics. Besides synthesis of co-ordination complexes, research involves studies of interactions with targets such as RNA, DNA and proteins, and often industrial and international interdisciplinary collaborations.

Research
Our current research projects include the following.

1. Design, synthesis and mechanism of action of transition metal compounds as photochemotherapeutic agents for the treatment of cancer. The aim of this work is to produce agents which can be activated by a range of wavelengths of light, are more selective for tumours, have less side-effects, and act by different mechanisms compared to existing drugs.

2. Design, synthesis and mechanism of action of organometallic anticancer complexes, including catalytic therapeutic agents. These compounds incorporate features for targeting and activation by a variety of pathways (e.g. aquation, ligand-centred redox processes, configurational changes)

3. Metal transport and delivery by the proteins albumin and transferrin, and the role of metal ions in neurological disorders.

These projects can involve use of a wide range of techniques and methods (e.g. synthesis, DNA assays, NMR, HPLC, UV-vis, CD, MS, x-ray absorption, photonics, microscopy, and cell biology, and interdisciplinary collaborations across physics, statistics, computation, biology, pharmacology, and medicine, depending on the interests of the research student.

Selected Publications
A potent trans diimine platinum anticancer complex photoactivated by visible light

Cytotoxicity, hydrophobicity, uptake and distribution of osmium(II) anticancer complexes in ovarian cancer cells
S.H. van Rijt, A. Mukherjee, A.M. Pizarro and P.J. Sadler

Penetrative DNA intercalation and G-Base selectivity of an organometallic tetrahydroanthracene RuII anticancer complex
H.-K. Liu, J.A. Parkinson, J. Bella, F. Wang, P.J. Sadler
Chemical Science, 2010, 1, 258 – 270.

Oxovanadium(IV) cyclam and bicyclam complexes: potential CXCR4 receptor antagonists
A. Ross, D.C. Soares, D. Covelli, C. Pannecoque, L. Budd, A. Collins, N. Robertson, S. Parsons, E. De Clercq, P. Kennepohl and P.J. Sadler

Controlling platinum, ruthenium and osmium reactivity for anticancer drug design
P.C.A. Brujininx and P.J. Sadler

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Research Summary
Metal complexes and their application to catalysis and materials, focussing on the synthesis of metal complexes using organic, organometallic and inorganic synthetic methods. Particular interest in chiral systems and the unique properties that they impart, and in the elucidation of synthetic mechanisms. Work applied to specific problems in areas such as enantioselective catalysis, chiral magnets and conductors and polymer synthesis. Techniques include vacuum line manipulations, gloveboxes, electrochemistry, crystallography, modern NMR, and electronic and other spectroscopies. Recent projects include enantioselective cyclo-hydroamination, new catalysts for polyolefins and copolymers, novel fuel additive technologies, magnetochiral anisotropy and the creation of stereogenic metal centres.

Research
Metallo-Organic Chemistry
We are a group of synthetic chemists working on a range of projects connected with metal complexes with a particular interest in chiral systems. Our research focuses on:

- design and synthesis of metal complexes with well defined chiral architectures
- enantioselective catalysis of organic transformations
- molecular materials such as chiral conductors and magnets
- bioinorganic chemistry based on optically pure water-soluble complexes for healthcare applications
- discovery of new catalysts and processes for the industrial polymerisation of alkenes

Selected Publications


Further Information
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Prof. Mike Shipman
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Professor of Synthetic Chemistry

Research Summary
The chemical synthesis of functional organic molecules underpins many key advances in human medicine, crop protection, biotechnology, and material science. Hence, the development of efficient, cost-effective routes to carbon-based molecules is an important, contemporary scientific challenge. Our research group specialises in this endeavour, pursuing the development of innovative synthetic methods alongside application-driven projects.

Current Research Projects
Work is focused on the development of new methods for the construction of organic compounds and their use in the preparation of a diverse range of functional molecules. The work is often collaborative. Illustrative examples included:
(i) the preparation of biologically active natural products and the study of their mode of action;
(ii) new agents for the treatment of pancreatic cancer;
(iii) the synthesis and evaluation of new materials that act as molecular switches;
(iv) the development of new multi-component reactions for the rapid and efficient assembly of biologically important molecules using strained heterocycles.
(v) the synthesis of new organic components for solar cells.

Selected Publications


Further Information
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Research

Femtosecond spectroscopy
The interaction between femtosecond laser pulses (1 femtosecond=10^{-15} seconds) and molecules has attracted considerable interest in recent years. The ability to follow chemical reactions using such ultrafast laser pulses led to the 1999 Nobel Prize in Chemistry to Ahmed Zewail for his work on transition states of chemical reactions using femtosecond spectroscopy. Ultrafast lasers can be used as very fast cameras, allowing experimentalists to take snapshots of processes such as energy transfer in molecules. One example of this process is molecular bond dissociation. By observing how bonds are broken and formed, this can lead to very detailed insight into the mechanisms of chemical reactions.

Pump-probe spectroscopy
Femtosecond pump-probe spectroscopy enables us to follow in real time vibrational motions coupled to electronic transitions. If the system is excited by a laser-pulse shorter than the vibrational period, the vibrational coherence that is induced in both the ground and excited states provides detailed information about the nuclear dynamics of the excited state.

In a pump-probe experiment, the output pulse-train from an ultrafast laser is divided into two beams, the pump and probe beams. A pulse train, (the pump) excites the sample and the changes it induces in the sample are probed by the second pulse-train (the probe), which is suitably delayed with respect to the pump. Some property related to the probe (e.g. absorption or ionization) is then monitored as a function of the time delay to investigate the photochemical changes triggered by the pump in the sample.

Our research uses two very powerful time-resolved techniques. The first is time-resolved mass spectroscopy (TR-MS) and the second is time-resolved velocity map ion imaging (TR-VMI).

Selected Publications

Active participation of πσ* states in the photodissociation of tyrosine and its sub-units, A. Iqbal and V.G. Stavros, JPC Lett., 2010, 1, 2274.

Further Information

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Dr Manuela Tosin
Laurea in Chemistry (cum laude), University of Padova, Italy; PhD, University College Dublin, Ireland; MRSC.
Assistant Professor of Organic Chemistry

Research Summary
Organic chemistry, protein chemistry, enzymology, microbiology and molecular biology, with the aims to
1) uncover the mechanisms involved in natural product biosynthesis;
2) generate novel natural products of improved pharmacological activity;
3) develop inhibitors of pathogenic microorganisms.

Research Statement and Interests
I recently joined the Chemical Biology Research Cluster at the University of Warwick, Department of Chemistry (November 2010). My research focuses on the application of synthetic chemistry to solve biological problems, such as the isolation and characterization of transient chemical species from the biosynthesis of natural products. Natural products are an invaluable source of therapeutic agents for human, animal and plant diseases; however they can also be implicated in the pathogenesis of infectious diseases and cancer.

As chemists we develop simple but innovative methods to investigate Nature’s ways and their evolution. This knowledge can be then used to our advantage, for instance to engineer bacteria and plants to produce new and more effective antibiotic and anticancer agents, or to design and prepare synthetic inhibitors of virulence factors.

My research addresses these issues and is highly interdisciplinary, as it spans from synthetic and analytical chemistry, to protein chemistry, structural biology, molecular biology and (bio)activity screening. Specific research interests are:

1) The development of synthetic probes of natural product biosynthesis.
2) The development of small-molecule inhibitors of biosynthetic processes.
3) Combinatorial biochemistry.
4) The chemistry and the biochemistry of glycosyltransferase enzymes.
5) The chemistry and biology of nitrogen-fixing bacteria and plants.

Selected Publications


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Dr. Alessandro Troisi
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Professor of Physical Chemistry

Research Summary
Physical/theoretical chemistry, including: electron transport in molecular junctions; organic materials for electronics; coupling between electronic and nuclear motions in several contexts (spectroscopy, charge transport); complexity and self-organisation. A broad range of computational chemistry methods is employed but the focus is on the theories linking computable quantities with experimental observables.

Overview
We study various interesting physical properties of molecules and materials, developing theoretical models and applying computational methods (quantum and classical). We are interested in charge transport in organic materials and molecular junctions, charge transfer reactions and modelling molecular self-assembly.

Research
Charge Transport in Organic Semiconductors
One of the greatest challenges of material science is to build a wide range of organic materials for application in electronics. These include light emitting diodes for displays and lighting, and thin film transistors for cheap circuits. Good materials for organic electronics should have high charge mobility, but the factors limiting the charge mobility are not well understood for this class of compounds. We investigate the theory of charge transport in ordered organic, trying to adapt standard computational methods and developing new transport models. We recently suggested that the proper mechanism to describe charge transport in organic crystal is diffusion limited by thermal off-diagonal disorder [28]. Under the funding of EPSRC these concepts are currently extended to the study of semiconducting polymers.

Selected Publications


Further Information
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Research Summary
We develop new and unique techniques that can visualise interfacial processes and phenomena that are difficult to see with other approaches. From electrocatalysis to living cells, from the growth of crystals and minerals to the function of new materials, such as carbon nanotubes and graphene, we seek to discover new aspects of interfacial processes and new interfacial phenomena that have not been observed before. Our philosophy is to think creatively and to do imaginative experiments, coming up with new instruments, applications and analysis in a multidisciplinary environment. As well as uncovering fundamental processes, our research is of considerable interest to world-leading companies with whom we have partnerships.

Research
Our research seeks to develop and apply new paradigms for interfacial processes which are of widespread fundamental and practical importance across the whole of science. Our approach is multidisciplinary, involving a large and diverse team with a variety of skills in the chemical, physical and life sciences, and involves the development of leading edge high resolution quantitative imaging techniques which are used to investigate a diversity of processes - for example: cell-membrane transport (biomimetic models and live cells); the growth of crystals, minerals and biominerals; and electrode reactions (e.g. at carbon nanotubes, graphene and in electrocatalysis), among many possible applications. When appropriate, our experimental work is underpinned by modelling of mass transport and chemical reactivity. We are very well funded and have an impressive multidisciplinary infrastructure, further enhanced by key collaborations, including several state of the art AFMs, two laser scanning confocal microscopes, and many unique high resolution electrochemical imaging workstations which we have developed for which we are world-leading.

Our research is supported by the European Research Council Frontier Research Programme (2010-15), the EPSRC and many multinational companies (e.g. Unilever, Lubrizol, Syngenta, GSK, BP, E6) and we have a close partnership with the UK's National Physical Laboratory.

Selected Publications
Evanescent wave cavity-based spectroscopic techniques as probes of interfacial processes
Scanning Electrochemical Microscopy as a Quantitative Probe of Acid-Induced Dissolution: Theory and Application to Dental Enamel
Localized High Resolution Electrochemistry and Multifunctional Imaging: Scanning Electrochemical Cell Microscopy
Probing Redox Reactions of Immobilized Cytochrome c Using Evanescent Wave Cavity Ring-Down Spectroscopy in a Thin-Layer Electrochemical Cell
Intermittent Contact–Scanning Electrochemical Microscopy (IC–SECM): A New Approach for Tip Positioning and Simultaneous Imaging of Interfacial Topography and Activity
Fabrication of Versatile Channel Flow Cells for Quantitative Electroanalysis Using Prototyping
Kinetics of Porphyrin Adsorption and DNA-Assisted Desorption at the Silica–Water Interface
Electron transfer kinetics at single-walled carbon nanotube electrodes using scanning electrochemical microscopy

Further Information
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Dr. Richard I. Walton
MA (Oxon) PhD (Reading) CChem MRSC
Associate Professor of Inorganic Chemistry

Research Summary
Development of new synthetic methods for the production of novel inorganic materials. Control of crystal chemistry and crystal form in one step synthesis for tuning the properties of complex materials. Transition-metal oxide materials with properties that may be applied in electronic and catalytic applications. Porous materials and their properties. Understanding the crystallisation of solid-state materials using novel in-situ probes, particularly time-resolved powder diffraction. Characterisation of the solid-state using powder X-ray diffraction. Use of synchrotron X-ray and neutron scattering and spectroscopy methods at central facilities.

Research
Our research lies in the interdisciplinary area of solid-state materials chemistry. We are interested in the synthesis of inorganic solids, their structural characterisation and measurement of their properties. We actively collaborate with industry to investigate applications of the materials we prepare: for example, currently with Johnson Matthey plc and Gyproc (part of Saint Gobain). Structural characterisation is performed in house using powder X-ray diffraction (including a high temperature chamber and a reactive gas cell), thermal analysis, and electron microscopy (in collaboration with the Department of Physics at Warwick). We also make extensive use of central facilities for structural characterisation, including the DIAMOND (UK), HASYLAB (Germany) and ESRF (France) synchrotron facilities, and the ISIS (UK) and ILL (France) neutron sources.

Four areas are currently under investigation:

Materials Synthesis
Transition-Metal Oxide Materials
Zeolites and their Analogues
Metal Organic Framework Materials (MOFs)

Selected Publications


Further Information
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Research Summary
Synthetic chemistry and asymmetric catalysis; Enantioselective ketone reduction using transfer hydrogenation and asymmetric carbon-carbon bond forming reactions using homochiral transition metal catalysts; Total and partial synthesis of natural products; Development of catalysts for hydrogen generation; Development of supported reagents for synthesis. Our group use a wide range of structural and analytical techniques such as infra-red, NMR, mass spectrometry, X-ray diffraction and atomic absorption spectroscopy.

Research
Key areas of research include:
- Organometallic asymmetric catalysis of organic reactions and, in particular, asymmetric transfer hydrogenation of ketones and imines.
- Novel synthetic methodology for complex molecule synthesis.
- Organocatalysis of organic reactions.
- Generation of hydrogen gas from biomass materials.

Asymmetric Catalysis of Organic Reactions
Recently we have published on asymmetric organometallic and organocatalysis of asymmetric reactions, and hydrogen generation from formic acid. Some examples are shown below:

Selected Publications
'Kinetic and structural studies on 'tethered'Ru(II) arene ketone reduction catalysts' Fung Kei (Kathy) Cheung, Adam J. Clarke, G. Clarkson, David J. Fox, Mark A. Graham, Changshee Lin, Andriana Lorente Civillé and Martin Wills, Dalton Trans. 2010, 39, 1395 - 1402.


Inhibition of Prolyl Oligopeptidase using a Synthetic Unnatural Dipeptide, Daurgirdas T. Racys, Dean Rea, Vilmos Fulop and Martin Wills, Bioorg Med. Chem. 2010, 18, 4775-4782.


Further Information
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