

FACULTY OF
SCIENCE



THE UNIVERSITY OF
SYDNEY

2010 SCHOOL OF CHEMISTRY RESEARCH REPORT



“Of all the subjects I studied here at Sydney, I loved Chemistry the most and had always intended to major in chemistry, and potentially pursue further study in it.”

MELLODEE ANVIA
HONOURS STUDENT

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ADVICE TO POSTGRADUATE STUDENTS

The University of Sydney's school of chemistry is one of the largest chemistry departments in Australia with a strong record of achievement and an international research reputation. There are typically around 100 postgraduate students undertaking research towards doctorate and masters degrees.

The school offers postgraduate programs in all areas of contemporary chemistry leading to the following degrees:

- Master of Science (MSc)
- Doctor of Philosophy (PhD)
- Graduate Diploma in Science (equivalent to 4th year of a BSc degree).

The school welcomes expressions of interest from both Australian and international students to undertake a postgraduate degree in chemistry.

All information on how to apply for candidature, scholarships, research projects in the School of Chemistry and other information for both Australian and international students may be found at:

sydney.edu.au/science/chemistry/study/postgraduate.html

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WELCOME HEAD OF SCHOOL



Professor Gregory G. Warr
Head of School
School of Chemistry

It is perhaps unsurprising when seeking themes for the School's research activities in 2010 that sustainability and the environment emerges strongly. Many research groups made important advances in the fundamental and applied chemistry of solar energy conversion, of water, hydrogen and carbon dioxide capture and storage, in biofuels, and developing greener, more sustainable chemical processes. These numerous and diverse achievements reflect one of the enduring characteristics of research in chemistry; solutions to current and relevant problems developed from a fundamental understanding of molecular structure, properties and transformation.

It might seem trite to call chemistry "The Central Science," but it is a cliché with a sound basis. Our sustainability research includes collaborations with engineers in academia, government, and industry. Another strong theme is biomedical research, including new drug leads and synthetic methods, controlled-release and targeted drug delivery systems. This involves extensive collaborations with the faculties of Medicine and Pharmacy, as well as with industrial partners in Australia and internationally.

From another perspective, both sustainability and biomedical incorporate elements of a strong nanoscience theme that pervades the School, incarnated in studies of polymers, biomaterials, amphiphiles, interfaces, framework materials, colloids, and crystalline and amorphous solids. Our leadership in many of these areas is built on our collective expertise and experience with major national and international research facilities including the Australian Synchrotron and ANSTO Opal research reactor, as well as international collaborations and facilities such as the Australian National Beamline in Japan, the US NIST Center for Neutron Research, and the UK's Rutherford-Appleton Laboratory.

The School of Chemistry's research philosophy is that all academic staff are supported to be research active, and to

be leaders in their field. Collaborations within and beyond the School can form and dissolve dynamically in response to the changes in common interests. Individuals thus unburdened by internal hierarchies have a particular agility and responsiveness to newly-emerging intellectual challenges and opportunities. Our research capacity is substantially enhanced by dedicated, high-level professional and technical expertise and facilities for NMR Spectroscopy, Mass Spectrometry, Vibrational and Optical Spectroscopy, X-ray Crystallography, Separations, Thermophysical Properties, and High-Performance Computing.

While our own undergraduate students continue to be the lifeblood of our outstanding cohort of research students, our international research student numbers are also a significant factor in both quality and our continually growing reputation in the region. In addition to the 123 postgraduate research students in the School in 2010, there were 31 Honours students undertaking year-long, research-intensive training, as well as numerous undergraduate scholars completing Talented Student Program research projects and summer research scholarships. In 2010 the School maintained its strong publication record, producing 1 book, 6 book chapters, 184 research papers and 40 refereed conference papers. Our research publications continue to be directed towards highly-ranked international journals. Staff and research students maintain our significant presence at national and international conferences. I thank our alumni/ae and donors for their generous support, particularly of postgraduate research scholarships and travel grants.

In 2010, members of the School received over \$6.6M in new research funding, leading to a total of 31 Discovery Grants, 7 Fellowships and 4 Linkage Grants from the Australian Research Council, totaling (with other grants) \$10.6M in competitive research funding. Our research continues to receive national and international recognition including NSW Young Tall Poppy Award to Dr Richard Payne, the Coblenz Award for molecular spectroscopy to Timothy Schmidt, and the election of Professor Jeff Reimers as a Fellow of the Australian Academy of Science.

Professor Greg Warr
Head of School

DR ROBERT W BAKER

ASYMMETRIC CATALYSIS

Planar-chiral half-sandwich complexes for asymmetric catalysis (*Radzey, Ward*): Asymmetric catalysis is one of the most active areas of current research in organic chemistry. Planar-chiral cyclopentadienyl metal complexes feature amongst the most successful asymmetric catalysts, but they are often very difficult to prepare in enantiomerically pure form. We have devised a new type of chiral cyclopentadienyl ligand, incorporating axial chirality, which allows the direct preparation of planar-chiral metal complexes in enantiomerically pure form. Most recently we have prepared a series of rhodium (III) half-sandwich complexes incorporating planar-chiral indenyl ligands with either thioether or sulfoxide pendant donor groups. The complexes are all readily prepared in enantiomerically pure form, and as single diastereoisomers in the case of the sulfoxide-appended ligands. We will be investigating potential applications of these and related complexes (in particular ruthenium (II) complexes) in a range of catalytic asymmetric transformations. We are also currently investigating the preparation of related tripodal ligands, where a third donor group is tethered to sulphur, with the aim of generating stereospecifically chirality at the metal centre. (See Figure 1)

Electron-rich monocyclic triarylalkoxyhydridophosphoranes (*Bacskaý*): In the course of the synthesis of an indenyl-phosphine ligand we isolated, not the expected indenol-phosphine intermediate, but the P(V) closed-chain tautomer **1**. There has been only one other report of such an electron-rich monocyclic triarylhydridophosphorane, compound **2**, described by Goldfuss *et al.* in 2001. These authors carried out calculations [ONIOM(B3LYP/6-31G*:UFF)] that indicated that the open-chain P(III) tautomer of **2** was

>19 kcal/mol more stable than the closed-chain P(V) tautomer. Accordingly, they proposed that compound **2** was "metastable". We have carried out calculations without use of the ONIOM method [B3LYP/6-31G(d)] and this indicates that the P(III) open-chain tautomer of **2** is only favoured by 0.25 kcal/mol. We have also synthesised the phosphine **3** (R = Me) and observed a small amount (*ca.* 10%) of the closed-chain P(V) tautomer, which ³¹P DNMR studies have shown is in equilibrium with the P(III) form. We are currently synthesising a series of compounds **3**, with varying R groups, in order to probe both experimentally and theoretically the factors responsible for the position of this equilibrium. (See Figure 2)

Figure 1

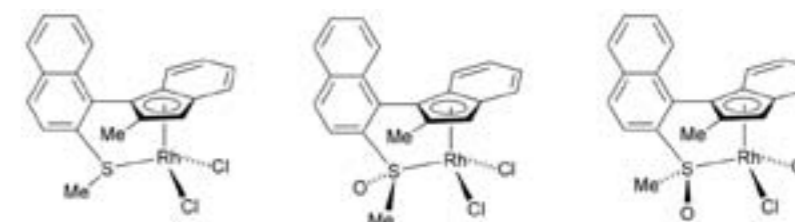
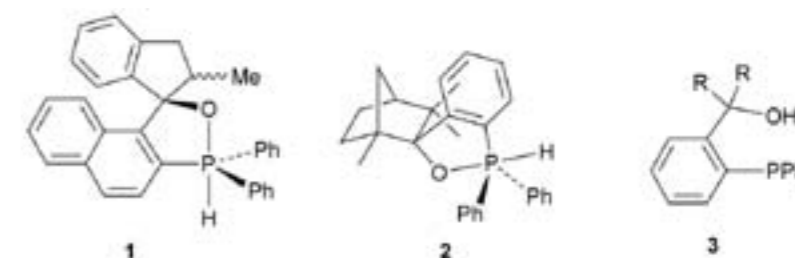


Figure 2



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ASSOCIATE PROFESSOR JAMES K BEATTIE

With Angus Gray-Weale we have developed an explanation for certain properties of water at hydrophobic interfaces. We are now exploring some of the profound implications of this model.

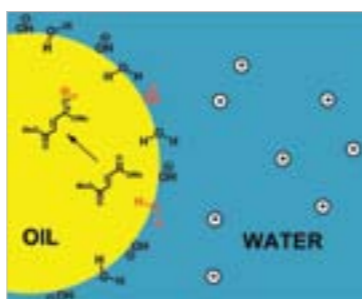
WATER AT HYDROPHOBIC INTERFACES

Hydroxide ion adsorption (*Gray-Weale, Djerdjev*): It has been known for 150 years that air bubbles in water are negatively charged. From the pH dependence of their zeta potential it was inferred that the charge is due to the adsorption of hydroxide ions. Similar effects are observed with oil drops and inert surfaces such as Teflon, which imply that the charging is a property of water, and not of the hydrophobic material. No molecular explanation for this effect was available. Our model is illustrated below. In bulk water the fluctuations of the molecular dipoles become correlated, leading to an attractive force, analogous to the van der Waals force which arises from electronic fluctuations. Ions negate this attractive force because the water molecules within their hydration sphere are constrained and cannot participate in correlations with the surrounding bulk water molecules. This unfavourable effect can be minimized if the ion moves close to the interface with a low per-

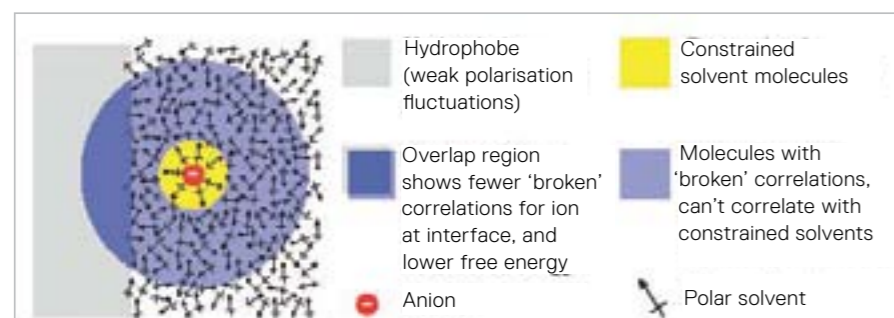
mittivity material, for then fewer bulk water molecules are adversely affected. This force attracts all ions to hydrophobic interfaces, but the hydroxide ion is particularly strongly adsorbed because it has a large dielectric decrement, and is small enough to get close to the interface to reduce the number of bulk water molecules affected.

The hydrophobic effect (*Djerdjev*): Other ions with large dielectric decrements should also adsorb in competition with the hydroxide ion. One such is the tetrabutylammonium cation. We have been able to prepare positively charged hexadecane-in-water emulsions with $[\text{Bu}_4\text{N}]\text{Br}$ at pH <6. This cation is considered to be 'hydrophobic', but the hydroxide ion is not. The recognition that the adsorption of both can be explained by the same model suggests that the model contains the basis of the explanation of the general hydrophobic effect.

On-water catalysis (*McErlean, Phippen*): In 2006 Sharpless described the acceleration of some organic reactions with water-insoluble reagents by



formation of oil-in-water emulsions. McErlean recognised that all the reactions that are so enhanced occur by acid-catalysis. At first this appears paradoxical, as the surface of the oil/water emulsion contains adsorbed hydroxide ions. We developed the explanatory mechanism illustrated that is consistent with all of the available evidence. Water itself provides the proton for the acid catalysis. Its acidity is enhanced by the strong adsorption of the hydroxide ion at the interface. This enables acid catalysis to occur in neutral solution, a phenomenon with many potential applications.



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COMPUTATIONAL INORGANIC CHEMISTRY AND EDUCATION

Computational study of polyoxometalates: Polyoxometalates are a huge and structurally diverse class of compounds with remarkable but poorly understood chemical and physical properties. They are prototypical of the highly praised nanomaterials, displaying a versatility that raises interest in various domains of catalysis, magnetism, medical biology and functional materials. Their diversity, size and complexity make rational design of functional nanomaterials a real challenge.

We have published the first studies of their vibrational spectra and fundamental studies of their electronic structure. With Australian Research Council (ARC) funding, we are currently developing a global framework for predicting their structures and spectroscopic properties. This approach uses genetic algorithms and neural networks to process, locate and analyze the very many minimum energy structures that are possible for these large and highly flexible clusters. This is enabling us to probe

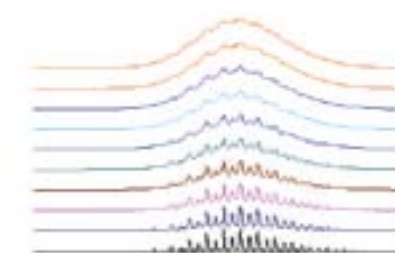
the interactions of these clusters with biomolecules and identify the structural and chemical basis of their medicinal and catalytic properties. Figure 1 shows the Keggin anion which is built from edge and corner sharing octahedra. The octahedra are slightly distorted, leading to low basicity on the surface and complex interactions with organic and bioorganic counter ions.

The electronic structure of transition metal and high temperature molecules:

We use density functional theory to model the structures, energetics and spectroscopy of transition metal complexes. For example, we have recently developed a method for calculating the polarized ligand-field spectrum of transition metal complexes with applications in bioinorganic and organometallic chemistry. This model allows us to accurately model the vibrational fine structure, band shape and intensity of linearly and circularized spectra of known molecules and to predict these features in the spectra of active sites in metalloenzymes. Figure 2 shows the variation in the ${}^1A_{2g} \leftarrow {}^1A_{1g}$ band in $[\text{PtCl}_4]^{2-}$ with temperature, modelled

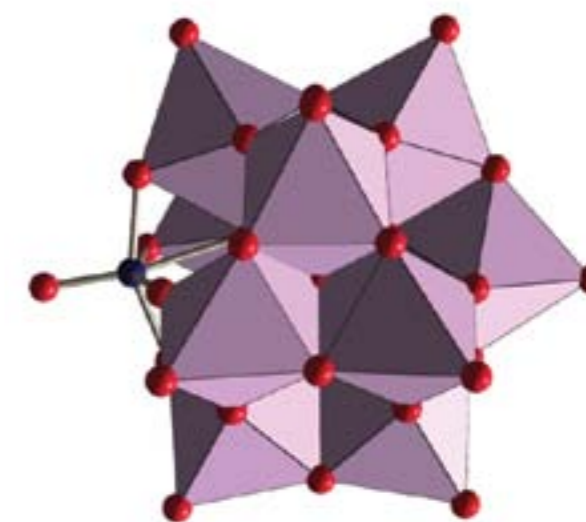
using density functional calculations which include spin-orbit coupling.

Figure 2



Chemical education: We are involved in a number of University and nationally funded projects designed to enhance chemical education and the student experience. These include ALTC funded projects in active learning in science and language difficulties in first year science education. We have been awarded University funding for projects developing generic attributes and the scientific method in first year science courses and a Vice Chancellor Award for Support of the Student Experience for the development of software to deliver rapid and personalized feedback.

Figure 1



PROFESSOR JOHN CANNING

INTERDISCIPLINARY PHOTONICS

The interdisciplinary Photonics Laboratories carry out research in all aspects of photonics, particularly those in novel material systems and applications.

Self-assembled photonics: A recent breakthrough has been a novel method of self-assembling silica-based photonic wires which can be doped with almost any material, including organic dyes and functionalised porphyrins, demonstrated by student Masood Naqshbandi. In contrast to existing methods involving the drawing down of optical fibres, self-assembly opens up a more practical approach to the fabrication of large quantities of wires for photonic applications ranging from micro and nano wire links of potential use in photonic chips to waveguide wire sensors with high evanescent field interaction. The use of various dopants permits nonlinear as well as linear optical properties to be enhanced and characterised. Other possible applications include improved solar cell performances using these structures.

FTIR microscopic studies by student George Huyang with Dr. Petermann have allowed improved titania layers to be deposited onto substrates – titania is increasingly important given its potential compatibility with optical waveguides, especially in nanolayer form, and its superior bio and chemical activity, allowing ready integration of materials onto silica and silicon, the two key platform materials. Several orders of magnitude improvement in sensor design was achieved using self-assembled

titania within a structured optical fibre. Novel surface functionalisation has also enabled a new approach to fabricating gold fractal layers for potential plasmon generation to enhance a number of processes, including fluorescent biodiagnosics markers.

Masood Naqshbandi also demonstrated using inkjet technology novel control of self-assembled mesostructured silica spheres doped with various materials, including graphene and laser dyes.

Laser processing of materials: In 2011 the presence of molecular O₂, postulated to be released during plasma generation in glass using femtosecond lasers, was confirmed using the Raman microprobe facility within the Vibrational spectroscopy laboratories. Both free and solvated forms of molecular oxygen were detected under typical processing conditions used to create porous nanogratings in irradiated glass. UV laser induced fluorescence of non-bridging oxygen hole centres within femtosecond written structures was shown to also be anisotropic, dependent on the polarisation of the laser by visiting student Maxence Rollin, from the Universite de Paris Sud. This in turn correlates with anisotropic propagation differences in waveguides written under similar conditions.

The regeneration process we developed earlier was taken a step further by showing that hydrogen was not required in the initial laser "seed" writing phase but essential in the regeneration phase. Using this knowledge, and in collaboration with the Institute of Photonics in Jena Germany, on-line single-shot laser pulse written tower fibre gratings were successfully regenerated by post-H₂ loading, elevating the temperature performance of these grating to 800 °C. This is another demonstration of laser

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spatially determined relaxation of glass permitting advanced functionalisation of glass potentially in all dimensions. In parallel with this activity, work with colleagues in India saw regeneration undertaken in different specialty fibres, both standard and fabricated at CGCRI Kolkata, to rule out the role of dopant diffusion in this process.

In 2010-2011, we demonstrated further how acoustic waves excited along a silica optical fibre can be used to alter the induced index change during holographic inscription of periodic structures into glass using UV laser light. Complex gratings ranging from sampled structures to Moire gratings, and a novel long period viscometer, were demonstrated by student Roberston Oliveira.

In 2011, we demonstrated, through an industry project with Thales Australia and the School of Physics, an improved interferometer for measuring ultra narrow linewidth lasers (<1kHz) and developed new approaches to enhancing detection sensitivity of optical hydrophone arrays. The techniques allow unprecedented direct linewidth measurement and noise studies that can benefit many sensor applications.

Roberston Oliveira (centre) wins Best Student Presentation at APOS 2010 for his work on a novel compact viscometer, helping to bring the conference to Australia in 2012, the first time outside of China (www.apos.2012.org)



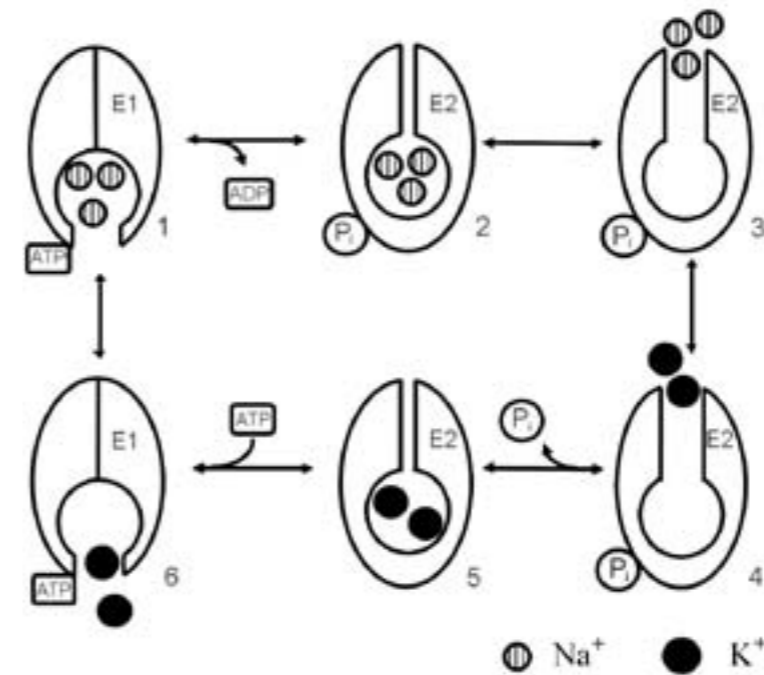
DR RON CLARKE

BIOPHYSICAL CHEMISTRY OF MEMBRANES

Mechanism of the Na⁺,K⁺-ATPase (Khalid, Myers, Noske, Fouassier, Cornelius¹, Apell²): The Na⁺,K⁺-ATPase, which is found in the plasma membrane of all animal cells, utilizes the free energy derived from ATP hydrolysis for the transport of Na⁺ ions out of and K⁺ ions into the cell. The concentration gradients of Na⁺ and K⁺ thus generated across the cell membrane have numerous important physiological functions, e.g. maintenance of the resting potential in nerve cells, cell volume regulation and nutrient reabsorption in the kidney. The aim of this project is to determine the kinetics and thermodynamics of the individual reaction steps of the enzyme's complex reaction cycle and thus obtain a deeper understanding of the mechanism of ion pumping and how it is coupled to ATP hydrolysis. Major tools involved in these investigations are stopped-flow fluorescence spectroscopy, which allows conformational changes and

charge translocation steps of the enzyme to be resolved on the millisecond timescale, and isothermal titration calorimetry, which can resolve the heat released in individual reaction steps.

Recently we discovered that mammalian kidney Na⁺,K⁺-ATPase occurs in the membrane in dimeric form. This allows the enzyme to have two gears of ion pumping depending on the ATP concentration. The protein-protein interactions within a dimer also increase the enzyme's ATP affinity and allow it to function more efficiently at low oxygen levels. In further studies on Na⁺,K⁺-ATPase from a cold-blooded animal (shark) we found no evidence for the dimeric form. Whether the enzyme occurs as a dimer or monomer thus depends on the animal species, and is possibly determined by body temperature. This work on protein-protein interactions within the Na⁺,K⁺-ATPase was recognized by the Australian Society for Biophysics with the award of the inaugural McAulay-Hope Prize for Original Biophysics.



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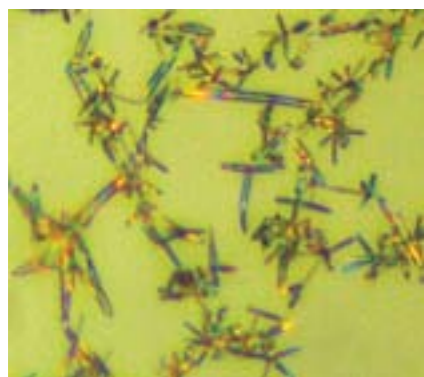


In detailed studies on the role of ATP in the enzyme's mechanism we discovered that ATP can bind to both unphosphorylated and phosphorylated forms of the enzyme. Apart from allowing the phosphorylation reaction itself to occur, ATP has allosteric effects on several of the enzyme's partial reactions. We were able to identify dual mechanisms by which ATP accelerates a conformational change of unphosphorylated enzyme, by abolishing steric hindrance within a protein dimer and by increasing the conformational flexibility of a monomer.

Using a recently purchased isothermal titration calorimeter (ITC) we developed a new method of following the steady-state kinetics of the Na⁺,K⁺-ATPase via the heat it generates during ATP hydrolysis. The method has significant advantages over colorimetric, enzyme-coupled or radioactivity-based assays, which have been the most commonly used methods in the field up to now. Our new ITC method doesn't require the addition of any extrinsic probes or enzymes, and for the researcher it avoids any health hazards associated with radioactivity-based methods.

¹University of Aarhus, Denmark
²University of Constance, Germany

PROFESSOR MAXWELL J CROSSLEY, FAA



SYNTHESIS OF FUNCTIONAL ORGANIC MOLECULES

Efficient photochemical up-conversion by triplet-triplet annihilation (Cheng, Roberts, Khoury, Fückel, Clady, Tayebjee, Ekins-Daukes*, Schmidt): Ring annulation of the pyrrolic rings of porphyrins leads to very interesting compounds that behave as π -expanded systems. These compounds have been found to behave as very efficient sensitizers for energy upconversion whereby a stream of light of a given photon energy is converted into one of a higher energy. Very efficient red to yellow light, red to green, red to blue, and green to blue upconversion has been demonstrated in our studies. A series of novel bis-porphyrin sensitizer molecules were prepared and their use as sensitizers is under investigation.

Porphyrins in structured optical fibres (Canning, Huyang, Naqshbandi, Boskovic): Compounds that form highly ordered monolayers on the interior of optical fibres were synthesized and studied. A new acid sensor was developed and meso-structured silica and titania particles were constructed.

New advanced materials (Holmes*, Wong*, Webb, A. Sum, Reimers): The design and synthesis of new advanced materials based on metalloporphyrins was continued. A porphyrin-hexabenzocoronene-porphyrin triad has been

synthesised, with its photophysical properties and performance analysed using a photovoltaic device. Studies in the areas of molecular switching devices and novel molecular circuitry were continued.

Synthesis and photophysics of models for the photosynthetic reaction centre (Lee, Reimers, Fukuzumi*, Ohkubo*, Wu*): Tris- and tetrakis-porphyrin chemical mimics of the chromophore arrangement of the photosynthetic reaction centre (PRC) have been further studied. The kinetic and thermodynamic properties of the synthetic PRC's were investigated using ultrafast and ESR spectroscopy and electrochemistry. More elaborate models that incorporate an additional C-60 acceptor unit were designed and synthesised. These are the closest mimics of the natural systems to be developed anywhere.

Porphyrins on surfaces (Martelli*, Kristensen*, Gibson*, Elemans*, Panduwinata, Chin, Reimers, Martelli*, Canning, Huyang): Studies on trialkylporphyrins [(C_nH_{2n+1})₃-NO₂P] have shown that the length of the alkyl chains and the deposition surface largely influenced the optical properties and microrod self-assembly. Trialkylporphyrin (C₅ to C₁₁) microrods that formed upon their deposition onto silica (α -quartz) were observed to have an average length of $\sim 0.7 \mu\text{m}$, and range in length from 11 to 170 μm . Trialkylporphyrins with much longer alkyl chains (e.g. C₁₉) typically formed powders. Interestingly, microrods formed from (C₇H₁₅)₃-NO₂P on silica also showed marked iridescence (shown in picture). Microrods formed from (C₇H₁₅)₃-NO₂P deposited onto silicon produced longer curved microrods with no iridescent character.

Porphyrin analogues as *Gingivitis* inhibitors (Yap, Simpkins, Collyer*, Hunter*): The black-pigment, Gram-negative bacterium *Porphyromonas*

gingivalis has an absolute requirement for either hemin or hemoglobin as growth factors. A series of porphyrin-antibiotic and porphyrin-amino acid-antibiotic conjugates and analogues containing biotin were prepared and used to further define requirements for recognition by HA2 receptors of the gingipains and to explore transport and in-cell processing.

Steroid bioconjugates (Taba, M. Sum): Porphyrin-steroid and porphyrin-sugar conjugates were synthesised and found to permeate A549 (human lung cancer) cells. Bioaccumulation was followed by confocal microscopy. Various water-soluble porphyrin-estradiol adducts were prepared for cell recognition studies.

Molecular recognition using porphyrins: development of a new histamine receptor (Chan*): Adopting the rarely used β -functionalisation strategy in porphyrin based sensor design, an amine receptive site was appended onto a zinc(II) porphyrin molecular framework affording a ditopic chemosensor – which selectively interacts with histamine in toluene via a 'two-site' binding mode (association constant $\sim 2 \times 10^6 \text{ M}^{-1}$). Spectroscopic methods and molecular modelling have established the viability of such a binding model.

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FUNCTIONAL INORGANIC MATERIALS

Our research spans the areas of inorganic chemistry, physical chemistry and materials science and focuses on the development of functional inorganic materials which exhibit novel electronic, optical and magnetic phenomena. Potential applications range from the capture of greenhouse gases to sensors, optoelectronics devices and photocatalysis. The key aspect is gaining an understanding of the fundamental relationships between the structural features of the solution- and solid-state materials and their physical properties.

Carbon dioxide capture (Das, Maj): The development of more efficient processes for CO₂ capture is considered a key to the reduction of greenhouse gas emissions implicated in global warming. In collaboration with Professor Jeff Long at the University of California, Berkeley, we have developed techniques for grafting amines onto highly porous three-dimensional solids known as metal-organic frameworks (MOFs) for use as CO₂ capture materials. A major achievement

has been the first successful design and synthesis of an air and water stable alkylamine-appended MOF which exhibits the highest heat of adsorption recorded to date for CO₂ in a nanoporous material due to the strong and selective interactions between alkylamines and CO₂ (which is the basis of current industrial capture processes in power plants using alkanolamine solvents). The results are significant in terms of revealing a class of materials with excellent CO₂ capture properties under realistic conditions in power plant flue gas. Our ultimate goal is the development of industrially-viable materials which can be readily integrated into industrial processes.

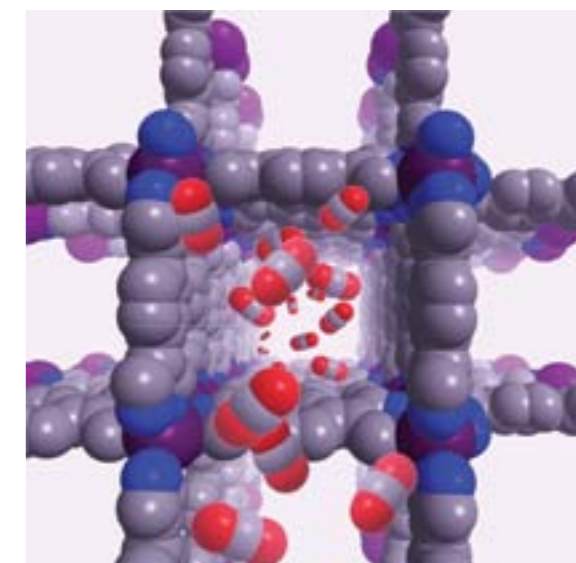
Microporous conductors (Kepert, Kanga, Caddy, Usov): Our work involves the design and synthesis of MOFs which exhibit the highly sought-after property of redox-activity (i.e. electronic conductivity). Recently, we have developed a series of frameworks based on the ruthenium cluster [Ru₂(CH₃COO)₄]^{0/+}, of which only one example had been reported previously. Solid-state electrochemical and spectroelectrochemical techniques are being developed to investigate the conductivity properties.

Our future work will involve the integration of mixed-valence metal clusters of Mo, W, Os and redox-active bridging ligands into MOFs to amplify their conductivities, as well as the integration of spin centres. In the latter case, we seek to explore the interplay between electronic and magnetic phenomena in such systems. The opportunities for advances at a fundamental and applied

level are immense, with potential applications ranging from sensors to molecular electronics devices.

Photoactive molecular sieves (Caddy): Recently, methodologies for the postsynthetic covalent functionalisation of MOFs have opened up fascinating prospects for building complexity into the pores. Our work involves the synthesis of materials as "photoswitchable molecular sieves" in which light can be used to modulate the size and polarity of the pores. Our strategy has involved the postsynthetic grafting of light-responsive organic molecules onto the interior scaffolds of MOFs. In order to establish a 'proof-of-concept' for the function of these new materials in gas separations processes, we have successfully synthesised three MOFs and are working towards the postsynthetic attachment of light activated molecules. We have also commenced work on the design of a combined irradiation and gas sorption apparatus to investigate the dependence of porosity on the wavelength of light irradiation.

Figure: Carbon dioxide diffusing through a porous metal-organic framework structure



DR ADRIAN GEORGE

In our current research we are interested in developing analytical methods sensitive enough to detect doping in competitive sport and to identify the origin of illegal drug seizures.

SYNTHESIS AND ANALYSIS

Detection of steroid use in sport (*Brooker, Cawley*): Improved High-Performance Liquid Chromatography - Tandem Mass Spectrometry (LC-MS/MS) methodology for the quantification and confirmation of synthetic glucocorticosteroid (GCs) abuse in sport has been developed and validated. Utilizing stable isotopically labeled processed internal standards, the method was used to assess excretion studies from permitted (topical/local) and prohibited (systemic) modes of therapeutic synthetic GC administration. Results from four forms of topical/local administration (dermal, inhalation, nasal spray, heel injection) of the synthetic GC triamcinolone acetonide (TA) showed that all TA excretion was completed within 24 hours, except for the injection study where detection was confirmed for up to four days post-administration. Results from an oral (systemic) administration of triamcinolone (T) showed that the maximum urinary concentration was greater than 3 µg/mL, or more than 100 times the World Anti-doping Agency

(WADA) specified (laboratory) minimum required performance limit.

Adrenosterone is an endogenous steroid hormone that has been promoted as a dietary supplement capable of reducing body fat and increasing muscle mass. It has been proposed that adrenosterone may function as a specific inhibitor of the 11β-hydroxysteroid dehydrogenase type 1 enzyme (11β-HSD1) that is primarily responsible for re-activation of cortisol from cortisone. The urinary metabolism of adrenosterone was investigated by gas chromatography-mass spectrometry (GC-MS) and gas chromatography-combustion-isotope ratio mass spectrometry (GC-C-IRMS). The exogenous origin of the most abundant adrenosterone metabolites was confirmed by GC-C-IRMS analysis with reference to urinary steroids from separate metabolic pathways. To develop anti-doping screening and confirmation criteria, GC-MS and GC-C-IRMS data from a reference population consisting of urine samples from 85 elite athlete volunteers was collated for comparison. As the analytical techniques used in this study are available to World Anti-doping Agency (WADA) accredited laboratories

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worldwide, the proposed criteria may be able to be efficiently implemented for the doping control of adrenosterone.

Profiling of synthetic illicit drugs

(*Salouros*): Trace impurities in clandestine manufactured drugs are the result of a number of reasons. They can be due to impurities being present in the precursors, solvents and/or reagents which can be carried over into the final product unchanged or they can react and be transformed into other products. Impurities can also be generated as by-products in the drug manufacturing process. Finally the conditions of storage, such as exposure to light and heat, as well as cutting agents introduced may affect the drug and/or impurities, thus introducing new impurities. Research is being undertaken to link the impurity profile in a reaction with method and conditions of synthesis. This will enable a 'finger print' of a synthetic approach to be established and, ultimately, provide a method to determine the origin of batches of seized drugs. More recently isotope ratio mass spectrometry has been applied to the profiling of methylamphetamine synthesis and is able to provide valuable information on the origin of the ephedrine or pseudoephedrine precursors.



PROFESSOR TREVOR HAMBLEY

MEDICINAL INORGANIC CHEMISTRY

Monitoring the penetration and effectiveness of anticancer drugs in solid tumours (*Byrce, Di Marco, Kim, Klein, Lo, Yamamoto, Zhang*): A limiting factor in the effectiveness of current anti-cancer treatments is the inability of the drug to penetrate throughout the entire tumour at a concentration sufficient to kill all cells. The aim of this project is to develop 3 and 4-dimensional cellular models of solid tumours for use as model systems to study anti-cancer drug penetration and the effect of those drugs on cell status and viability. Our recently developed 4-dimensional cellular models of solid tumours that expressed a photoconvertible green fluorescent when the cell was under conditions of hypoxic stress was used to study the response of spheroids to established anticancer agents including doxorubicin and cisplatin. These studies showed that the hypoxic cells became

mobile following drug treatment and rapidly migrated away from the remains of the spheroid. Work was continued on the transfection with other genes and of other cell lines to produce additional models that reported on hypoxia, iron status, and cell cycle status.

Tuning the chemistry of platinum(IV) and cobalt(III), and iron(III) complexes for anticancer applications (*Bonnittha, Chen, Ereve, Gui, Norman, Yamamoto*): The preparation of charged complexes designed to establish whether it was possible to manipulate the uptake in different regions of solid tumours with lower pH was continued. Studies of cellular and spheroid uptake were undertaken for a range of cobalt complexes encompassing a range of charges and these showed highly selective pH dependent uptake (Figure 1).

Our newly developed methods for functionalising platinum(IV) complexes were used to produce novel complexes with a variety of groups in the axial sites including fluorophores and charged species. The strategy was successfully modified to give unsymmetric complexes in high purity allowing the inclusion of fluorescent and charged species in the same complex. The attachment of peptides to the axial sites of platinum(IV) complexes was further investigated and click chemistry strategies were developed.

Targeting of metastatic tumours using MMP binding agents

(*Doan, Green, Kassiou*): Almost all compounds used in the treatment of cancer cause serious side effects because they lack selectivity for tumours. However, the rapidly increasing knowledge and understanding of the differences between the chemistry and biochemistry of tumours and healthy tissues means that it is now possible to

envisage drugs that act selectively on tumours.

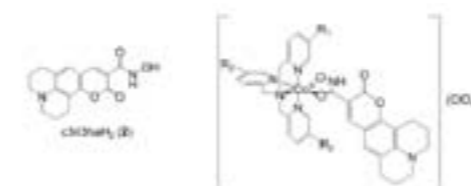
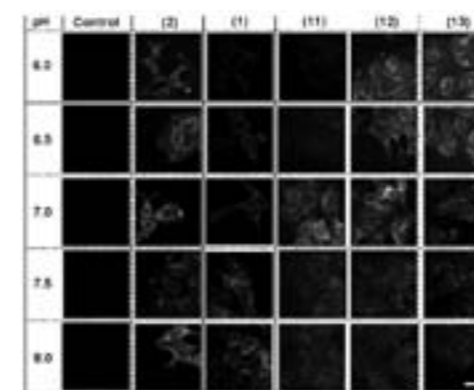
A set of 24 compounds was prepared with a range of groups chosen to impart selectivity in the binding to MMP-2, MMP-7, or MMP-9. Inhibition studies showed that most of the compounds were excellent inhibitors of one or more of these MMPs with IC₅₀ values ranging from the sub-nanomolar to low micromolar. Selectivity was achieved for MMP-2 and MMP-9 and relative selectivity was increased for MMP-7. Work was continued on the development of click chemistry radiolabelling methodologies and confirmed that this is a highly effective and efficient means of the 18F labelling of MMP inhibitors of the type we have developed.

Work was continued on the development of fluorescent rhenium complexes of MMP binding compounds so that in vitro work using ^{99m}technetium could be coupled with in vitro work using the rhenium complexes. A tumour cell migration assay was developed to monitor the impact of the MMP inhibitor on the metastatic behaviour of these cells and used to show that the inhibitors were effective in a live cell system.

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Figure 1. Confocal microscopy images of pH-adjusted DLD-1 cells after treatment with fluorescent cobalt(III) complexes for 4 hrs. Scale bar represents 20 µm.



R₁, R₂ = H: [Co(c343haH)(tpa)](ClO₄)₂ (1)
R₁ = COOH, R₂ = H: [Co(c343haH)(tpa(COOH))](ClO₄)₂ (11)
R₁ = H, R₂ = COOH: [Co(c343haH)(tpa(COOH))](ClO₄)₂ (12)
R₁, R₂ = COOH: [Co(c343haH)(tpa(COOH))](ClO₄)₂ (13)

PROFESSOR PETER R HARROWELL

I am interested in understanding how chemical structure, crystalline order and the miscellany of spatial patterns emerge spontaneously from the chaos of colliding molecules. The dynamics associated with such intricately correlated behaviour remains a major puzzle with significant practical consequences. My research involves using theoretical and computational methods to resolve the fundamental processes involved and to develop new and useful descriptions important aspects of the material world.

THEORETICAL CHEMISTRY

Ultrastable glass films and their odd behaviour on heating (*Leonard*): Recently, the group of Mark Ediger in Wisconsin discovered that ultrastable glass films could be made via vapour deposition just below the glass transition temperature. To achieve bulk glasses of similar stability would take over a million years. Given the importance of glass films in coating technologies and information storage, these experiments represent an important advance. We have developed the first comprehensive explanation of how these films are formed and how they behave when heated¹. Using a com-

puter model of a glass-forming liquid, we showed that the accelerated stabilization of the films is achieved because of the enhanced mobility of particles at the surface during deposition. One of the important results of our work was to establish that the behaviour of the glass films could be accounted just using aspects of cooperative relaxation already present (on a microscopic scale) in the bulk liquid without the need to add new surface-specific physics. This raises the prospect of using these films as a tool to study fundamental aspects of glasses.

The spatial distribution of dynamics near the glass transition (*de Souza, Canalier (Saclay), Widmer-Cooper (Berkeley), Douchot (Saclay), Biroli (Saclay), Reichman (Columbia)*): The study of the transient spatial pattern of kinetics in supercooled liquids near the glass transition has been responsible for the substantial advances in understanding the microscopic character of the slow dynamics responsible for the stability of amorphous materials. We have shown how mechanical constraints give rise to

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such dynamic heterogeneities and have used this picture to clarify their spatial character as the point of complete constraint is approached². The patterns of dynamics themselves evolve in time and we have established – both computationally and experimentally³ – how this evolution occurs in bursts, resulting in microscopic ‘avalanches’ of change in dense disordered materials

Geometry of stable structures in a supercooled binary alloy liquid (*Pedersen (Roskilde), Schroder (Roskilde), Dyre (Roskilde)*): Using computer simulations of the atomic dynamics in liquid alloy mixture, we have demonstrated that the liquid accumulated local structure similar to that of the crystal phase as it is cooled⁴. Employing the methods developed over 50 years ago to study complex inorganic crystals, we showed that the liquid structure could be characterised as a disordered network of Frank-Kasper bonds.

1. Leonard, S and Harrowell, P. *J. Chem. Phys.*, **133**, 244502, 2010.
2. de Souza, VK and Harrowell, P. *Phys. Rev. E*, **83**, 011501, 2011.
3. Canalier, R et al. *Phys. Rev. Lett.*, **105**, 135702, 2010.
4. Pedersen, UR et al. *Phys. Rev. Lett.*, **104**, 105701, 2010.

Time evolution of the Frank-Kasper network in a supercooled liquid alloy (ref.4)



ASSOCIATE PROFESSOR BRIAN HAWKETT

Our research is aimed at gaining an understanding of the factors governing the formation and stabilisation of colloidal dispersions so that we can use this understanding to solve scientific problems that are of interest to our industry collaborators.

POLYMER COLLOIDS

RAFT in disperse phase systems (*Neto, Nguyen, Aziz, Such*): Controlled radical polymerization allows a control of polymer and nanoparticle architecture that was previously only dreamt of. Reversible addition fragmentation chain transfer (RAFT) is the most versatile of the currently available controlled radical processes. In this broad based project with DuluxGroup Australia we exploit this new capability in our research to design and synthesize polymer particles and composite nanoparticles with particular emphasis on applications in surface coatings. Achievements in this project include the coating of individual unaggregated pigment particles with polymer to achieve improved pigment efficiency and thus reduce the amount required in a coating. Coating particles in this way has been a ‘Holy Grail’ of the coatings industry for many decades. Pigment efficiency has been still further improved by encapsulating individual pigment particles within hollow polymer particles, thus halving the amount of TiO₂ needed to achieve a given opacity. Also in this project, we have discovered a new approach to making Janus particles that enables their preparation both economically and on a large scale.

Polymer stabilisation of superparamagnetic nanoparticles for biomedical applications (*Hambley, Stephens, Jain, Pan, Pham, Bryce, Fong, Rozeleur, Tanudji, Jones*): In this project, a collaboration with Sirtex Medical Limited, we are using short chain amphiphilic macro-RAFT agent surfactants as anchored steric stabilisers for superpara-

magnetic nanoparticles. One objective in this project is to prepare microbeads (about 35 microns in diameter) that contain a high concentration (about 10⁹/bead) of individually stabilised magnetic nanoparticles that can be used for the hyperthermia treatment of liver cancer. The beads are of just the right size to lodge in the tumor when injected into the hepatic artery. The patient is then put in an oscillating magnetic field of appropriate field strength and frequency, causing the beads to heat up and destroy the tumor, with little collateral damage to other tissue. In another aspect of this collaboration we are studying the use of sterically stabilised nanoparticles to more efficiently treat cancers that involve solid tumors.

Inhibition of spontaneous detonations of explosive emulsions in hot reactive ground (*Beattie, Neto, Priyananda, Djerdjev, Gore*): In this collaboration with Dyno Nobel Asia Pacific we are gaining a fundamental understanding of the factors governing the interactions of explosive emulsions with hot and reactive ground. This understanding will allow us to devise strategies for the formulation of more stable explosive emulsions for use in hot and reactive ground.

Enhancing the efficacy and performance of agrochemical actives (*Perrier, Ali, Nguyen, Heming*): In this collaboration with Syngenta Crop Protection we are using controlled radical polymerisation techniques to provide more effective delivery systems for agrochemicals.

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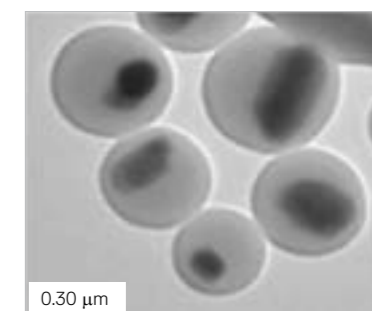


Figure 1: TiO₂ particles encapsulated by polymer

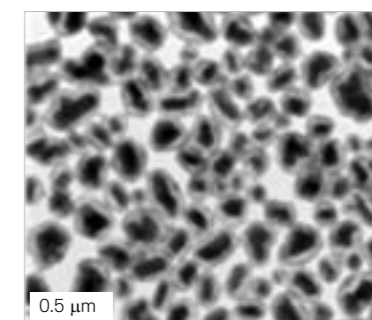


Figure 2: TiO₂ particles inside hollow particles

DR TOBY HUDSON

THEORETICAL MATERIALS CHEMISTRY

Structural search and dense packing (*O'Toole, Elias, Harrowell*): Packing models are increasingly being employed to predict and rationalize the architecture of metamaterials, self-assembled from nanoparticles, or colloidal crystals such as opals. We have developed a three-component systematic search methodology to find the densest structure for given particle shapes. Firstly, we have used the entire Inorganic Crystal Structure Database as starting points and representation classes for computer optimization. Secondly, we investigate categories of structures with interesting geometric motifs. Thirdly, we have developed a method of enumerating subspaces of the general search space. We have identified a number of densely packed structures that are not seen in atomic systems, as well as significantly improving the best known binary sphere packing for systems over large ranges of size ratio. The outcomes of this work include: an explanation for the observed size ratio of silica spheres in some precious opals; an argument that even after considering electronic effects in alloys with the NaZn_{13} structure type, the detailed structure is still principally determined by the solution to a sphere packing

problem; and, the first predictions of structures better than segregated close-packed lattices for all binary combinations with small sphere sizes of up to 65% of the size of the large spheres.

The approach used here, a combination of data mining and Monte Carlo simulated annealing, is a powerful tool for structural searches. We have begun applying this method to the design of materials with a range of geometric and functional properties.

Amorphous network relaxation (*Little, Chowdhury, Harrowell, Poole*): In contrast to crystals, where relaxation and diffusion mechanisms are dominated by the motion of discrete well-defined defects, amorphous materials often evolve using collective and unpredictable mechanisms. Unfortunately we cannot probe these complex events easily with experiment, because in glasses all we can usually get are averages and distributions. Computer modelling on the other hand has the ability to probe atomic and topological information directly.

We have studied a class of topology-altering mechanisms which can occur in any network, and represent a large fraction of the important dynamics for long-term changes in network glasses or liquids. These mechanisms can be

used to categorize observed topological changes, or as a broad set of trial moves that can be used in Monte Carlo simulations.

We used these mechanisms to study stress relaxation in networks like amorphous silicon, and supercooled liquid water. Stress relaxation is related to the viscosity of a material, and therefore is a key player in the transition from liquid to glassy behaviour. The simplest, and most commonly occurring of these mechanisms, irrespective of where it occurs in these networks turns out to cause a characteristic and predictable change in both the structure and stress. Furthermore, we find that local stresses have a role in selecting the likely sites for rearrangement events. These viscous liquids are starting to look less like a frantically chaotically tumbling mess, and more like a creaking Meccano structure where at any one time only particular joints are vulnerable to snapping, an earthquake which causes flow and aftershocks elsewhere in the system.

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Figure 1. An optimally dense packed structure with small spheres 65% the size of large spheres. This structure is thermodynamically stable without any interactions between particles.

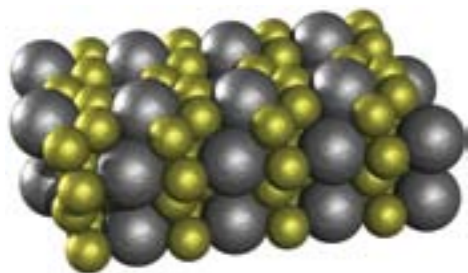


Figure 2. A low energy configuration of the continuous random network.



DR LUKE HUNTER

Our research focuses on the element fluorine, and on what happens when this extreme element is incorporated into organic molecules. A particular interest concerns the ways in which fluorine atoms affect molecular conformation. Understanding the conformational outcomes of fluorine substitution allows us to design shape-controlled molecules such as bioactive peptides for applications in medicine and biotechnology.

ORGANOFLUORINE CHEMISTRY

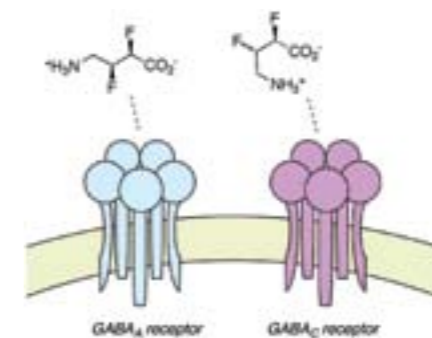
Fluorinated amino acids (*Cagnes, Jolliffe, Jordan*): We have developed methods to synthesise unusual amino acids that contain two adjacent fluorine atoms on the backbone. There are several possible stereoisomers, and we have achieved selective access to all of the isomeric forms of this molecule. We have shown that the different isomers have very different conformational behaviour: certain isomers have a rigid "linear" shape, while others exhibit conformational disorder and a "bent" carbon chain. These differences can be rationalised in terms of stereoelectronic effects associated with the C-F bonds. We have recently published these results in *Chemistry: A European Journal* and *Beilstein Journal of Organic Chemistry*. We are now focussing on incorporating these novel fluorinated building blocks into a variety of peptide systems that rely on conformation for optimal biological activity.

GABA receptor ligands (*Johnston, Collins-Chebib*): We are developing fluorinated amino acids as novel GABA receptor ligands, with potential applications in the treatment of epilepsy and insomnia. In collaboration with researchers in the Faculty of Pharmacy, we have identified molecules that show promising GABA receptor subtype selectivity. Some of these molecules are antagonists while others are agonists,

and these differences are attributed to the stereochemistry of the fluorination pattern and the way that this influences the ligands' conformation.

Cyclic peptide natural products (*Tai, Firth, Kirk*): We are investigating several cyclic peptide natural products including unguisin A (a marine-derived antibacterial agent) and pohlianin C (a plant-derived antimalarial agent). We are incorporating fluorinated amino acids into analogues of these molecules, and examining whether the fluorinated components can enhance the synthetic efficiency by preorganising the linear precursors into a "bent" shape that facilitates peptide macrocyclisation. In collaboration with biologists at The University of Sydney and at ANU, we are also probing the therapeutic

Figure 1: Fluorinated GABA analogues show shape-dependent receptor selectivity



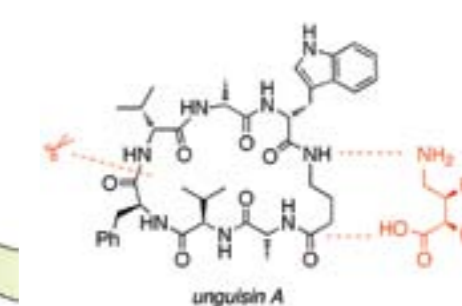
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potential of these fluorinated natural product analogues.

Fluorinated integrin ligands (*Ludbrook*): We have synthesised several fluorinated peptides that have been designed to bind selectively to integrin receptors in a shape-dependent fashion. In collaboration with GSK (England) we are investigating the integrin binding affinity and selectivity of these fluorinated peptides, with a view to applications in the treatment of cancer and thrombosis.

Figure 2: Fluorinated amino acids as turn-inducers to enhance cyclic peptide synthesis



PROFESSOR KATRINA JOLLIFFE

Our research focuses on using and developing the tools of organic synthesis for the development of molecules with a particular function. Specific targets include molecules capable of recognizing and sensing other molecules, and new antifungal drugs with a novel mode of action.

ORGANIC SYNTHESIS AND SUPRAMOLECULAR CHEMISTRY

Cyclic peptide based anion receptors (*Butler, Dungan, Young, Liu*): The selective recognition and sensing of biologically important anions under physiological conditions is of intense current interest to both chemists and biologists. Anions such as pyrophosphate ($P_2O_7^{4-}$, PPI) play important roles in bioenergetic and metabolic processes and the ability to selectively sense such anions has applications in biomedicine. Backbone modified cyclic peptides are ideal scaffolds for the construction of molecular anion receptors and we are currently investigating the synthesis and application of a range of such receptors. We have exploited the pre-organisation of the *Lissoclinum* class of backbone rigidified cyclic peptides to prepare a number of anion receptors. These bear side chains with either hydrogen bonding or metal ion binding sites for anions and in some cases show selective binding for pyrophosphate ions in physiological media.

Exploiting reversible turn-inducers for the efficient cyclisation of small peptides

(*Cochrane, Fairweather, Wong*): Naturally occurring cyclic peptides exhibit a wide range of biological activities and are often more resistant to enzymatic hydrolysis than their linear counterparts. Additionally, the restricted conformational flexibility of cyclic peptides allows them to present functional groups in a spatially well-defined manner and is of use in the study and mimicry of protein folding. However, the currently available methods for the head-to-tail cyclisation of linear peptides are often slow and low-yielding. We recently developed a new method for the efficient head-to-tail synthesis of small cyclic peptides and examined its use in a model system. We have now extended this methodology to the synthesis of novel cyclic peptides incorporating from 4-9 amino acids and have applied it in the synthesis of the anti-tumour cyclic peptide Axinellin A and in the synthesis of the core of LI-F04a, a cyclic depsipeptide with antifungal

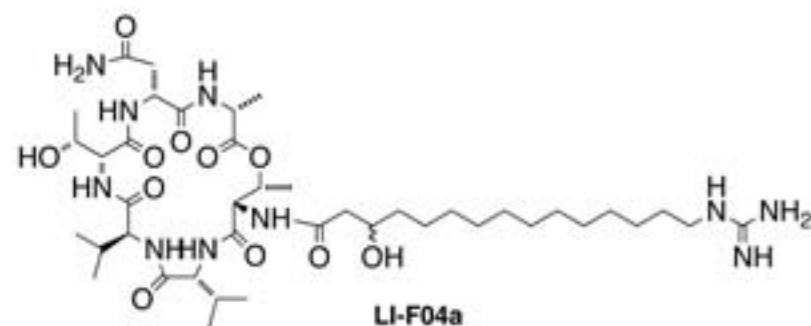
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activity. We have also expanded our methodology to synthesise all-L cyclic tetrapeptides in good yield.

Design and synthesis of antifungal agents with novel modes of action

(*Cochrane, Koda, Yoon, Sorrell*, Djordjevic**): Pathogenic fungi are increasingly implicated as a cause of serious and potentially fatal disease, especially in immunocompromised hosts. Current therapies are limited in safety and/or efficacy and resistant fungi are an emerging problem. The primary aim of this project is to design and synthesise novel antifungal agents with activity against key fungal pathogens and favourable pharmacokinetic and safety profiles. We have synthesised several classes of antifungal compounds with novel structures and assessed their haemolytic activity and cytotoxicity as initial indicators of safety. We have commenced work on determining the mode of action of these compounds, which appears to be different to those of currently used antifungal agents. Our best compounds have activity comparable to the gold standard of antifungal drugs, Amphotericin B and exhibit low toxicity towards mammalian cells. These compounds are promising lead structures for the development of new antifungal agents.



“After I finish my degree I am hoping to work as a postdoctoral researcher overseas with the ultimate aim of pursuing an academic career.”

CAMERON WEBER
PHD STUDENT



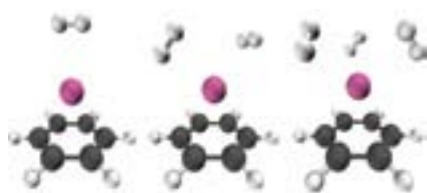
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INTERMOLECULAR INTERACTIONS

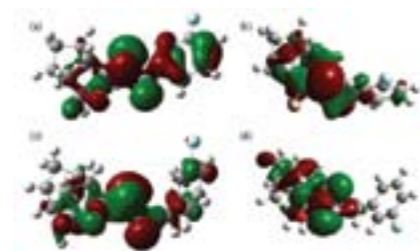
Potential energy surfaces (Kolmann, Morris, Collins (ANU), Gordon (Iowa)): Molecular potential energy surfaces (PES) describe how the energy of a molecule changes as its atoms move. We have developed new interpolation techniques for constructing PES based on *ab initio* quantum chemical calculations and have coupled these with iteration methods capable of growing a PES until the calculation of a given quantity has converged. Research into growing PES as efficiently as possible is ongoing and we are currently extending our *Grow* computer package to enable calculations on non-metallic crystalline materials.



Above: Equilibrium structures for one, two and three adsorbed H₂ molecules

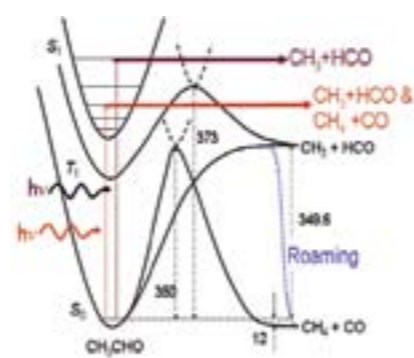
Hydrogen storage materials (Kolmann): Electronic structure calculations have been used to develop reduced-dimensional PESs for model systems that mimic H₂ adsorption in the Lithium-doped metallo-organic framework material (MOF-5).

Grow has been combined with quantum diffusion Monte Carlo (QDMC) simulations to predict vibrationally averaged (ground state) structures of adsorbed H₂. This has demonstrated that the H₂ molecule is delocalised over the organic fragment. We are currently developing path integral Monte Carlo techniques to investigate how the quantum nature of such systems changes with temperature.



Above: Minimum energy structures and HOMOs for 4 possible σ binding ligands

Reaction dynamics (Kable, Maccarone, Rowling, Heazlewood, Osborn (Sandia), Bowman (Emory)): In collaboration with experiment, the photodissociation dynamics of acetaldehyde, CH₃CHO, on both the S₀ and T₁ electronic PES has been studied. This has confirmed the presence of a newly discovered "roaming" reaction mechanism and demonstrated that it is much more complicated and ubiquitous than first envisioned. Our studies have also pinned down various experimental parameters for the acetaldehyde PES. In further experiments, electronic structure calculations and kinetic modelling we have explored the nature of the CD₃CHO PES and elucidated unexpected H/D isotope exchange.



Above: Schematic of acetaldehyde photodissociation

Computational drug design (Kassiou, Banister, Hunter, Jolliffe): Research has focussed on molecules active at central nervous system receptors.

Sigma receptors (Kassiou, Banister) exert a neuromodulatory effect in the central nervous system. Calculations on fluorinated derivatives of trishomocubane-derived hemiaminals, which have been shown, experimentally, to be highly selective at the two sigma receptor subtypes, have indicated that sigma binding affinity is largest for ligands where there is significant highest occupied molecular orbital (HOMO) character along the alkyl bridge between the hemiaminal and the fluorobenzene group, suggesting electrons are donated from this orbital into the lowest unoccupied molecular orbital (LUMO) of the receptor site. HOMO density on the aromatic ring (ie in the pi orbitals) reduces affinity for the sigma-receptor.

Sigma-aminobutyric acid (GABA) receptors (Hunter, Jolliffe) inhibit neuronal firing. Fluorinated GABA analogues have been made experimentally and calculations have been used to determine their stable conformers in aqueous solution and chloroform and to predict their NMR spectra. The presence of fluorine modules the molecular structure and leads to differing biological activity.

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LASER SPECTROSCOPY AND PHOTOCHEMISTRY

Unexpected and extensive photo-induced isomerisation (Jordan, Maccarone, Heazlewood, Andrews, Osborn (Sandia), Klippenstein and Harding (Argonne)): In 2010 we investigated photochemically-induced isomerization in acetaldehyde. The isomerization pathways were followed experimentally using specifically labeled reactants (CD₃CHO and CH₃CDO), and modeled by extensive transition state theory calculations. They reveal extensive and unprecedented isomerization of the reactant, before the final products emerge. The dominant products of bond fission are CD₃ + HCO, but we found that, remarkably, the relative yield of CD₂H + DCO products can reach about 20%. Such efficient isotopic scrambling was completely unexpected, but has now been explained by performing RRKM-master equation calculations on the best available, multidimensional ground (S₀) potential energy surface. These calculations identify a sequence of four elementary H/D shifts as the dominant exchange mechanism, with rate coefficients that are competitive with the C–C bond fission in both CD₃CHO and CD₂HCDO

— resulting in products that show significant isotope scrambling (Figure 1). At the longest wavelengths, the molecule isomerizes up to 20 times before the C–C bond breaks.

There are important implications for these findings. Until now chemical models of the atmosphere assumed a molecule emitted into the atmosphere stays fixed as that molecule until it is either photolysed (broken up) by sunlight, or attacked by other molecules. Our results show that this is not the case. Acetaldehyde itself is an abundant atmospheric pollutant. Atmospheric models of acetaldehyde dispersal include only photolysis and reaction with a small number of radical species. This work shows that up to 20% of CH₃CHO may undergo keto-enol isomerisation to CH₂=CHOH – a species with very different atmospheric rates and pathways. This work was submitted to *Nature Chemistry* in 2010 and published in 2011. (BR Heazlewood, et al., *Nature Chemistry*, 3, 443 (2011)).

The hydrogen bond in ammonia (Crim, Case and Heid (U. Wisconsin)): In 2010, I was on sabbatical at the University of Wisconsin, Madison, hosted by Professor Fleming Crim. Whilst there I worked on a variety of projects, including this project exploring the

hydrogen bond in ammonia. Hydrogen bonding in the second row hydrides, HF, H₂O and NH₃ are often used as examples of prototypical hydrogen bonds, and appear in most First Year Chemistry textbooks. The H-bond energy between two H₂O molecules is known to be with 0.1 kJ/mol, as is the (HF)₂ binding energy. However, the binding energy between two NH₃ molecules was only known to lie in the range 6.2 – 11.4 kJ/mol.

In these experiments, we prepared a molecular beam of NH₃, and (NH₃)₂ in Helium. The dimer was selectively excited by an infrared laser which provided enough energy into the dimer to fragment it into two monomers. Both the internal (vibration-rotational) energy, and recoil kinetics energy was probed using ion imaging (Figure 2). In the image, each ring corresponds to a different internal state of the NH₃ fragment, while the diameter of the ring is proportional to its kinetic energy. Conservation of momentum and energy allowed us to determine the strength of the H-bond between two ammonia molecules to be 7.9 ± 0.2 kJ/mol. The experiments also provided an insight into the way that the H-bond in ammonia is broken. Fragment molecules were observed with very high internal energy; states with high kinetic energy were significantly disfavoured.

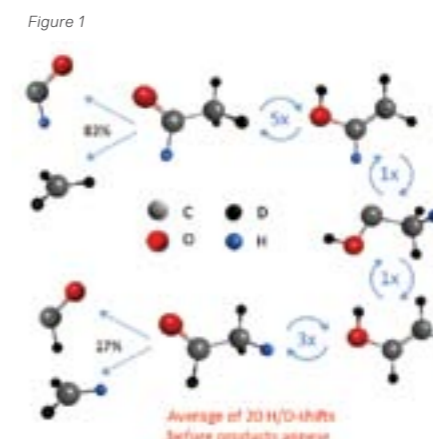
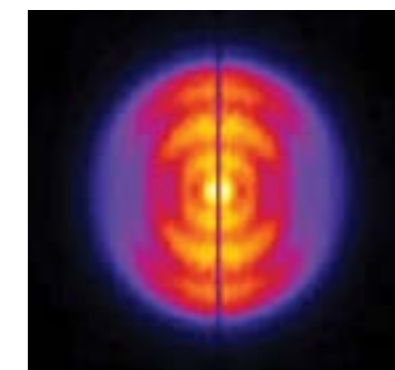


Figure 1

Figure 2



ASSOCIATE PROFESSOR MICHAEL KASSIOU

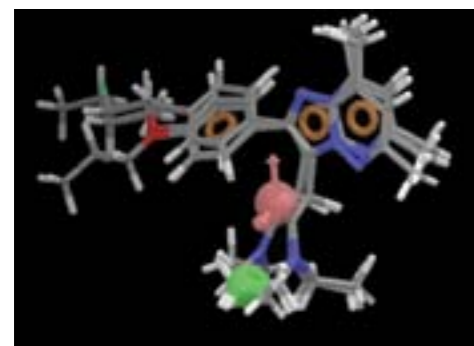
Our research focuses on the discovery, design and synthesis of bioactive CNS molecules. Understanding the interactions of these molecules with their biological targets as part of structure-activity relationships studies allows the rational design of more efficacious treatments for diseases of the brain.

DRUG DISCOVERY/MEDICINAL CHEMISTRY

Immunomodulation in the treatment and diagnosis of CNS disease (*Reynolds, Hanani*): The recognition that microglial activation is closely linked to the pathophysiology of brain disease has made the translocator protein (TSPO) an important therapeutic and diagnostic target. We have investigated the structure activity profile of molecules based on pyrazolopyrimidines and determined parameters required for maintaining high binding affinity based on an existing pharmacophore model. We have further refined this model by investigating the effects on nitrogen substitution within the heterocyclic scaffold. Although this is not considered in the pharmacophore model it has great impact on binding affinity of these molecules.

Purinergic P2X₇ receptor in depression (*Wilkinson, Schiavini*): Over the last two decades there has been increasing evidence of a strong

(TSPO pharmacophore hypothesis (AHRRR, where A = hydrogen bond acceptor, H = hydrophobic group, and R = ring system). Pink sphere – hydrogen bond acceptor, green sphere – hydrophobic group, tan hoop – ring system.



relationship between depression and immunological dysfunction in depressed patients. Excessive secretion of cytokines, such as interleukin-1 β (IL-1 β), and tumour necrosis factor- α (TNF- α) is increasingly recognised as a potential cause of depression. The purinergic P2X₇ receptor modulates the maturation and release of cytokines such as IL-1 β suggesting that the P2X₇ receptor could play a role in the pathophysiology of depression and that blockade of the P2X₇R might result in antidepressant-like properties.

To date, only a few classes of drug-like molecules are known to interact with the P2X₇R. We have developed a library of small polycyclic scaffolds with varying polycyclic hydrocarbon and aromatic segments, which are currently the subject of pharmacological studies in order to evaluate their antidepressant potential.

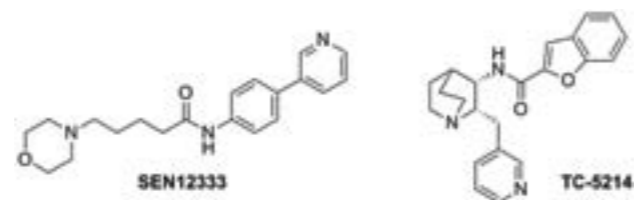
Chemistry and biology of nicotinic receptors (*Paine, Beinat*): Nicotinic acetylcholine receptors (nAChRs) belong to the family of ligand-gated ion channels which are regulated by acetylcholine, one of the major excitatory transmitters in the nervous system. The $\alpha 7$ nicotinic receptor subtype is particularly important in the potential treatment schizo-

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phrenia. We have developed structure-activity relationships strategies of the following small molecules (SEN12333 and TC-5214) in order to understand the motifs conferring $\alpha 7$ activity.

Chemistry of sigma receptors (*Banister, Moussa, Yoo*): Ligands which bind with high affinity at sigma receptors have been shown to modulate and interfere with several neurotransmitters and have potent activities in animal models suggestive of antipsychotic, cognitive enhancing, neuroprotective, and antidepressant activities. We have recently reported the synthesis and binding a novel series of trishomocubanes of the type 4-azahexacyclo[5.4.1.0^{2,6}.0^{3,10}.0^{5,9}.0^{8,11}]dodecane which display high affinity for sigma-2 and sigma-1 receptor subtypes respectively. These molecules have also been shown to modulate cocaine induced behaviours. These lead compounds provide the basis for further refinement of the binding and functional activity of this class.



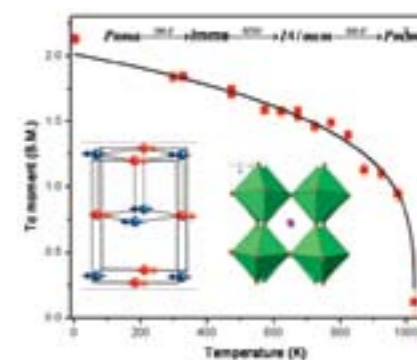
PROFESSOR BRENDAN KENNEDY

Our current research strives to understand the importance of local instabilities on the structures and properties of metal oxides. The motivation for this work is to discover new physical and chemical properties and to provide fundamental understanding to allow for the development of improved materials for applications in areas such as electronics and energy generation. Specifically we are interested in the effects of chemical substitutions on structural phase transitions, using variable temperature high resolution powder diffraction methods.

indicate that SrTcO₃ has G-type antiferromagnetic structure, in which each Tc moment is antiparallel to its six nearest neighbours, observed below. The magnetic structure is collinear antiferromagnetic with the technetium moments parallel to c-axis.

Orbital ordering in manganese perovskites: The oxidation states of both Ce and Mn in the series (Sr_{1-x}Ce_x)MnO₃ (x = 0.1-0.4) were investigated using Ce L- and Mn K-edge X-ray absorption near edge structure measurements. We have found that although Ce is predominantly 4+ at low doping levels (x = 0.1 and 0.15), the Ce valency decreases with increasing Ce doping (reaching a value around 3.5+ at x = 0.4). The average Mn oxidation state decreases with the increase of Ce content. High resolution neutron diffraction studies demonstrate the structures are tetragonal in *I4/mcm* for x \leq 0.30 and that although the octahedral tilt angle increases with increasing Ce content, the distortion of the MnO₆ octahedra is reduced significantly at x \geq 0.2 due to a transition from the long-range ordered Jahn-Teller distortions to incoherent static distortions.

A similar study of the series CaRu_{1-x}Mn_xO₃ with 0 < x < 1 using a combination of Mn K-edge and Ru L_{3,2}-edge X-ray absorption near edge structure spectroscopy and high resolution synchrotron X-ray powder diffraction also revealed complex electron transfer behaviour. The formation of Mn^{3+/4+} - Ru^{4+/5+} redox pairs accounts for the unusual chemical composition dependence of the cell volume, evident from the diffraction studies. The co-existence of mixed valence redox pairs is also believed to contribute to the phase separation observed at 0.1 \leq x \leq 0.6.



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SOLID STATE AND MATERIALS CHEMISTRY

Technetium oxides: We have recently embarked on studies of the structures of some technetium oxides. Extremely little is known regarding the structure and properties of technetium oxides, as a consequence of the absence of any naturally occurring Tc isotopes and the radioactivity of those available. Using a combination of high resolution neutron and synchrotron X-ray diffraction, supported by electronic structure calculations we have discovered unexpectedly high Neel temperatures in the simple perovskites CaTcO₃ ~ 800 K and SrTcO₃ ~1000 K. The latter is the highest observed magnetic transition for a 4d transition metal. At room temperature SrTcO₃ is orthorhombic as a consequence of cooperative tilting of the corner sharing TcO₆ octahedra. The tilts are sequentially removed as the sample is heated with the oxide displaying the sequence of structures *Pnma* \rightarrow *Imma* \rightarrow *I4/mcm* \rightarrow *Pm3m*. Neutron powder diffraction data collected in the temperature range 4-1023 K

PROFESSOR CAMERON KEPERT



MOLECULAR FRAMEWORK MATERIALS

Nanoporous molecular frameworks (*Southon, Price, Keene, Duyker, Chen, Chadbourne, Barkhordarian, Murphy, Peterson, McKenzie, Brown, D'Alessandro*): A range of new framework materials that display reversible guest sorption is being investigated. Characterisation of the dynamic host-guest structures of these phases using a broad suite of techniques, which include the *in-situ* measurement of single crystal and powder X-ray/neutron diffraction data during guest sorption in combination with gas/vapour sorption measurement, is leading to highly detailed structural and physical understandings of the novel host-guest chemistry of these phases. Of particular interest is the selective adsorption and storage of a range of technologically and environmentally important gases, which include H₂, CH₄, CO₂ and O₂. Our demonstration that bare metal sites provide optimal binding sites for volatile guests has paved the way to hybrid materials that are able to discriminate between such species highly selectively and store them under non-extreme conditions. Materials under investigation span a range of metal-organic framework materials through to sophisticated biomimetic systems capable of chemisorptive guest binding.

Thermal expansion *Wu, Duyker, Cameron, Chadbourne, Price, Kanga, Murphy, Phillips, Lock, Halder, Yuan, Chapman, Goodwin, Bridgeman, Peterson, Kearley*: Materials that shrink upon warming (negative thermal expansion; NTE) or that are temperature invariant (zero thermal expansion; ZTE) are of considerable fundamental interest due to their rarity and have diverse potential applications in thermal compensation. We have recently uncovered two very broad families of such materials: metal-cyanide frameworks and metal-organic frameworks. For the cyanide phases, we attribute the unprecedented NTE to two different modes of transverse motion of the linear cyanide bridge. For the metal-organic framework systems, both soft transverse phonons and, uniquely, local molecular vibrations are responsible for the anomalous expansion properties.

Switching nanoporous materials (*Price, Li, Goux, Sciortino, Southon, Fellows, Mullaney, Neville, Halder, Chapman, Murray, Moubaraki, Létard, Brooker*): Our incorporation of molecular electronic switches into nanoporous frameworks and discrete complexes is leading to materials and molecules that have unique physicochemical properties and potential applications in molecular sensing and data storage. Through the systematic variation of the ligands and

counter-ions we have developed an extensive family of materials of this type, allowing fine-tuning of guest-exchange (pore size and shape) and switching (transition temperature) properties. Of particular note is the recent generation of an array of Hofmann-type systems, which display highly novel guest sorption properties and hysteretic spin-crossover.

Electron localisation/delocalisation (*Keene, Kanga, Murphy, Price, Kurmoo, D'Alessandro*): In this project we are exploiting the versatility of molecular chemistry to incorporate a range of interesting electronic, magnetic and photochemical/photophysical phenomena into nanoporous materials. Of principal interest are magnetic ordering, electron delocalisation and photoactivation, with the goal being to create materials in which coupling with reversible host-guest function leads to entirely new materials properties. This work is opening new routes to explore the influence of structural perturbation on electronic/magnetic/photophysical properties and promises to underpin a range of future high-level applications, spanning molecular sensing, molecular electronics, batteries, selective electrodes and energy conversion.

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BIOINORGANIC CHEMISTRY

Anti-diabetic effects of chromium, vanadium, molybdenum, and tungsten (*Aitken, Carter, Finney*, Gasparini, Glover*, Levina, McLeod, Nguyen, Pham, Vogt,**): Empirical methods were employed to determine the structures and speciation of Cr and V complexes in biological fluids, cells, and tissues using linear combinations of XANES from model complexes that contain biologically relevant ligands. This was used to study the biotransformations of anti-diabetic drugs and supplements in gastrointestinal juices, blood and target cells. X-ray absorption mapping of protein gels of blood fractions or cell lysates was used to determine the proteins to which the Cr is bound and to examine the local environment of Cr within the bands using micro-XANES.

Further research has been conducted on the oxidation of Cr(III) dietary supplements to carcinogenic Cr(VI) by biological oxidants. A combination of vibrational microprobe techniques and immunoblotting assays have been used to provide evidence that Cr(VI), Cr(V), Mo(VI), V(V), W(VI) inhibit phosphatase enzymes within target adipocytes (fat cells), which is probably a major cause of the anti-diabetic activities of

Cr, Mo, V and W anti-diabetic supplements.

Ga, Rh and Ru anti-cancer drugs (*Aitken, Baker, Carter, Finney*, Glover*, Hambley, Harris*, Levina, Liang, Lim, Liu, Katsifis*, Nguyen, O'Riley, Tobin*, Vogt,* Wood*): Research has been conducted on Ru and Ga anti-cancer drugs using similar methodologies as those described above to study their biotransformations in biological fluids and cells.

Ru anti-cancer drugs undergo substantial aquation, hydrolysis and oligomerisation processes under physiological conditions and bind to various proteins and cells. The differences in reactivities of different drugs were explained by the kinetics of ligand-exchange reactions with respect to whether the drugs react primarily against extracellular molecules and cell membranes (anti-metastatic effects) or within the cell and cell membranes (cytotoxicity against primary tumours). A range of assays on adducts of Ru drugs with serum albumin have shown that these adducts are highly anti-metastatic. This is a very important result since up to 95% of Ru is bound to serum albumin (such adducts were previously thought to be inactive) on intravenous administration of certain drugs currently in phase 2 clinical trials.

Differences in the biotransformations of Ga pro-drugs are important in understanding their efficacies and safety. The speciation of different Ga pro-drugs in blood, gastric juices and cells was examined using X-ray absorption spectroscopy and radioisotopes.

As described for the Cr complexes, X-ray microprobe studies of protein gels were also used to further understand the speciation of these drugs in biological fluids and cells.

XAS studies of isolated and intracellular heme proteins (*Aitken, Austin*, Ball*, Hunt*, Witting**): XAFS studies

were conducted on various isolated heme proteins. The research involved: determining the structures of indoleamine 2,3-dioxygenase-2 that has recently been isolated from kidneys and is involved in blood pressure control, and H₂O₂ oxidized myoglobin. These studies have produced important new results on the functions and structures of heme proteins of relevance to a range of biological processes and diseases.

Disease diagnosis and differentiation in cells and tissues (*Aitken, Armstrong, Carter, Cohen,* de Jonge,* Double,* El-Assaad,* Gottlieb,* Grau*, Hackett, Hunt,* Lee, Levina, McQuillan,* Paterson,* Siegele,* Singharay, Vogt*): Vibrational spectroscopic diagnostics for various diseases including cerebral malaria, bacterial meningitis, viral meningitis, graft-versus-host disease and Parkinsons disease were investigated. Strong correlations were observed between these new diagnostics and standard pathology diagnostics and, in some cases, the vibrational spectroscopic techniques had the potential to enable disease diagnosis prior to any clinical effects. Such early diagnosis has considerable potential in improving the health outcomes and the University has gone into the national phases of patenting of the technology. Vibrational spectroscopic mapping and imaging were used, together with proton-induced X-ray emission (PIXE) and synchrotron X-ray microprobe techniques, to understand the biochemistry of cerebral malaria and meningitis.

Identification of ancient and extant microbes (*Aitken, Carter, de Jonge,* Edwards,* Emry,* Marshall,* Paterson,* Vogt**): X-ray microprobe data were analysed to identify ancient microbial fossils and to compare them with the signatures of extant extremophiles in research that is aimed at understanding more about the origins of life on Earth and to examine potential biomarkers of life on Mars.

DR CHRISTOPHER LING

MATERIALS CHEMISTRY; NEUTRON & X-RAY SCATTERING SCIENCE

The most important underlying principle in materials chemistry is that of “structure-property relations” – the idea that we can relate the crystal structure of a material to its chemical composition on the one hand, and to its physical properties on the other. A detailed understanding of structure provides a link through which we can use chemistry to manipulate and optimise the properties of functional materials.

The goal of our research is the discovery, characterisation and optimisation of functional solid-state materials. Structural characterisation plays a central role, and we make particularly heavy use of neutron, synchrotron X-ray and electron diffraction as well as complementary techniques such as spectroscopy and electron microscopy. Structural information is used to guide exploratory synthetic studies and to interpret the results of physical property measurements.

Solid-state ionic conductors

Solid-state ionic conductors are the performance-limiting components of emerging energy technologies such as solid-oxide fuel cells and lithium-ion batteries. The materials currently used are quite simple – they have small unit cells with high symmetries, which are

partially disordered at ionic conducting temperatures. Examples include yttria-stabilised zirconias in fuel-cell membranes and lithium cobaltates in battery cathodes. Some more complex materials show better performance under ideal conditions, but they are too unstable for practical applications. A major impediment to improving their performance and stability is a lack of detailed understanding of the atomic-scale mechanisms responsible for their properties.

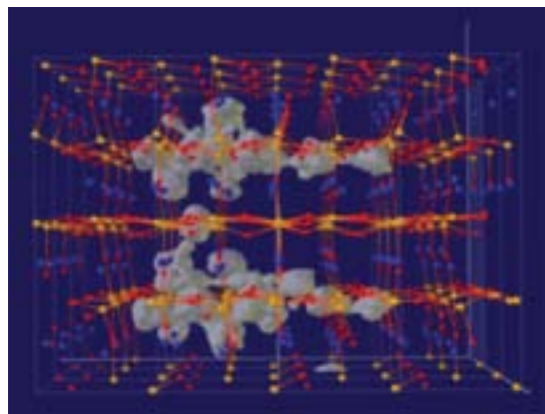
In 2010 we published our findings on several new complex solid-state ionic conductors, revealing their unusual crystal structures and conduction mechanisms on an atomistic level. This includes a new series of mixed oxide ionic, protonic and electronic conductors $Ba_4(Nb,Ta)_2O_9 \cdot xH_2O$. Both the Nb and Ta compounds undergo reconstructive phase transitions at $\sim 1200^\circ C$ from a common low-temperature phase to completely different high-temperature phases. The quenched high-temperature form of $Ba_4Nb_2O_9$ is particularly interesting as it hydrated stoichiometrically ($x = 1/3$), giving rise to 2D layers built of NbO_4 tetrahedra and discrete OH groups that allow fast ion conduction.

We are now beginning to expand the scope of our studies from structure to dynamics, using a combination of

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ab initio (density functional theory) molecular dynamics calculations and inelastic/quasielastic neutron scattering experiments to gain insight into ionic conduction mechanisms. This is a particularly powerful approach in systems where we can grow large (cm-scale) single crystals for the experimental component using our floating-zone image furnace.



PROFESSOR THOMAS MASCHMEYER

ADVANCED CATALYSIS FOR SUSTAINABILITY

Sustainable chemistry and processes: The world is standing at the technological threshold of a revolution that is driven by the need for truly sustainable (industrial) processes, both in the production of chemicals as well as in the generation of power.

At current rates of resource usage, a world population operating with Australian standards of living would require between 4 – 6 planets. Clearly, this is untenable and, from a chemical viewpoint, the inherent challenges can only be met by devising strategies for increased use of renewable resources, waste reduction, energy optimisation and process intensification as outlined in the 12 principles of “Green Chemistry”.

Our group aims to tackle these issues and *enhance sustainability by generating and using new fundamental insights on the molecular and nanoscopic level to develop feasible leads for the design of new catalytic chemical routes and processes.*

Renewable chemicals and fuels:

We model the processing of carbohydrates, lignins and lignocellulosic biomass in *state-of-the-art* continuous flow reactors (in a joint effort with Prof. Brian Haynes at Chemical Engineering). Sophisticated physical techniques are used to identify reaction products and obtain reaction kinetics. Design and synthesis of model compounds also play a significant part of the projects. Some of the questions we want to answer are:

- Can we influence carbohydrate decomposition pathways in water such that the onset of decarboxylation (the main pathway for biomass de-oxygenation) can be clearly delineated?
- What are the linkages in lignin that are most susceptible to

hydrolysis in super-critical water? Can we predict whether certain biomass feedstocks are better or worse suited to hydrothermal upgrading?

- Is it possible to achieve hydrogen transfer and subsequent de-oxygenation via *in-situ* generated formates?

Aqueous phase reforming: Recently, Dumesic reported a most unusual observation – the generation of alkanes from sugar in water. The micro-kinetics of this extremely complex reaction system are increasingly well understood. However, the catalysts used function well only in the absence of sulphur. Imparting sulphur resistance while maintaining catalytic performance is the key target of this project. Our main approach is via the synthesis of multimetallic nanoparticles in which various catalytic properties can be tuned. Success would allow ordinary cellulosic materials to be turned into alkanes in water in one step. Activities in this area involve inorganic synthesis and characterisation as well as catalytic testing and sophisticated analyses by gas chromatographic and mass-spec techniques.

Ionic liquids as novel synthesis media:

Ionic liquids are experiencing boom-times – why? Increasingly it is becoming clear that this most versatile group of liquids has very special properties that are most likely rooted deeply in their ‘saltiness’, i.e. their large degree of organisation, even in the liquid state. Projects in this area involve the synthesis and characterisation of ionic liquids as well as the evaluation of chemical selectivity that can be imparted by them onto various chemical conversions. Some of the questions we are trying to answer are:

- Can we delineate a relationship between observed changes in reactivity and presumed structural

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features of ionic liquids?

- What are the key structural features that have the most impact?
- Can we design ionic liquid systems for particular conversions?

Photocatalysis: hydrogen from water:

Although this reaction has been proven to work – it is still a long way from being effective enough to be useful. Here, we aim to prepare new materials, based on the band-gap engineering of self-assembled nanostructures to provide better catalysts for this reaction. Our focus lies on dispersed, TiO_2 -stabilised exotic multicomponent nanoparticles and coupling these to reducing ‘sacrificial’ solutions that enhance the thermodynamics of the system. Such solutions can be readily found in the environment where they often present problems. Our approach yields hydrogen from water using sunlight and as a ‘spin-off’ improves the water quality by oxidising smelly and toxic species such as sulphides.

ASSOCIATE PROFESSOR TONY MASTERS

ORGANOMETALLIC CHEMISTRY AND CATALYSIS

If we are unable to hand to our children, and to their children, the means to at least as good a lifestyle as that we now enjoy, we have failed miserably as a civilisation. This challenge becomes more acute as we approach the resource and energy limits of our planet.

To even approach a “sustainable” existence, such that the ecosphere exists in a “steady state” able to support our current lifestyle, a 4 to 10 fold increase in the resource efficiency of existing production processes will be necessary. In the longer term, this will involve the development of a suite of novel industrial chemical transformations, such as those envisaged in the biorefinery. However, in the short term, small absolute improvements to large scale existing processes can have maximum impact. Our research embraces both approaches, involving for example, fundamental studies of workhorse reactions, such as catalytic hydrogenations, as well as the development of improved catalysts for existing process, such as hydrocarbon oxidations. In applied studies, we collaborate with local industry to develop an Australian manufacturing capability for novel “ionic liquid” solvents. Representative projects are described below.

Hydrocarbon oxidation catalysts: One of the most fundamental industrial petroleum-based operations is the catalytic selective oxidation of hydrocarbons to produce materials such as epoxides, ketones, aldehydes, alcohols, acids, and derivatives of these molecules. These account for some 25% of industry’s monomer and chemical intermediate production, annually generating in excess of \$B50 of business roughly equally across America, Europe and Asia. As a consequence, oxidation catalysts rank second only to polymerization catalysts in industrial usage. In many cases, the oxidant is chlorine or

organic peroxides. We have developed novel hydrocarbon oxidation catalysts, capable of delivering significant gains in resource efficiency.

Catalytic properties of silica surfaces:

Within the high technology world of advanced materials, one simple stoichiometry reigns supreme – SiO₂. Silica dominates the field of catalysis, as supports, shape selective catalysts, Lewis and Brønsted acids and as crystalline, amorphous, structured amorphous, microporous, mesoporous and macroporous solids, or, “simply” as surfaces. Silica occupies an equally dominant position in electronic and optical devices. Silica is conventionally presumed to be an “inert” catalyst support, however, we have shown the silica surface, once thermally activated, to be an excellent catalyst for the production of high quality polymers. Our work has also focussed on the understanding of this effect by examining the reaction chemistry of silsesquioxanes – molecular models of fragments of the silica surface.

Nanotherapeutics: The delivery and release of drugs specifically to the disease site remains one of the great challenges of modern chemotherapies. Many drugs suffer from a lack of specificity, resulting in a systemic distribution of the drug, which attacks both healthy and diseased cells with consequent deleterious side-effects. We are attempting to solve this problem by using nanoparticles as generic drug delivery platforms, able to convey a drug to a disease site, releasing the drug only when within that site. Nanoparticles are particles small enough to enter cells, and chemical functional groups capable of binding chemotherapeutic agents are readily attached to their surfaces.

New high performance zinc bromine batteries with novel electrode/electrolyte systems: Australia has substantial wind and solar resource capabilities,

however they are being harnessed on only a small scale. Efficient energy storage is a missing link for renewable energy. Zinc-bromine batteries have great potential as energy storage devices due to their high theoretical power density. They suffer however from serious drawbacks mainly related to bromine solubility and volatility. In collaboration with local companies, Alpha Chemicals and ZBB, and Professor Tony Vassallo (Chemical and Biomolecular Engineering) our group is redesigning the existing system by introducing a combination of mesoporous materials and ionic liquids. A new zinc-bromine cell will possess enhanced power density and will be safer to use compared to the old system. Our research is directed at creating high performance energy storage devices which will help to utilize renewable energy sources more efficiently.

Other projects include novel catalysts for remediation of non-potable water supplies, the development of new, high surface area solids as catalysts and catalyst supports, catalysts formed by molecular imprinting, novel catalysts through nanoencapsulation, and sulfur tolerant reforming catalysts.

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DR CHRISTOPHER MCERLEAN

Advances in all aspects of chemistry are reliant on our ability to build new molecular entities in a timely, efficient, economically sustainable and environmentally benign manner. Our research group is addressing this challenge by investigating new reactions and applying known reactions in novel settings to access molecules that display biological promise.

SYNTHETIC ORGANIC CHEMISTRY

Intramolecular Stetter reaction to access polycyclic ethers (Goldys):

Polycyclic ethers are a class of natural products isolated from the marine algae responsible for ‘red-tide’ events. Some of these structurally imposing molecules have been identified as causative agents in mass outbreaks of seafood poisoning, but other members of the class, (such as protoceratinII) display beneficial properties. To date, however, the potent anti-tumour, anti-fungal, and anti-cystic fibrosis activity of polycyclic ethers has been poorly studied due to difficulties in isolating or building the desired molecules.

We have recently disclosed our solution to this problem which involves the use of an intramolecular Stetter reaction to rapidly generate arrays of polycyclic ethers in a stereocontrolled fashion. Efforts are underway to generate a library of analogues in order to elucidate the structural features responsible for the biological activities of this class of compounds.

The McErlean group



Enantiocontrolled access to oxygenated tetrahydrofurans (Nesbitt):

Tetrahydrofuran rings that have an oxygen atom attached at the 3-position are a commonly encountered structural motif; they are present in natural products from the terrestrial and marine environments (such as kumausallene) as well as being present in some pharmaceuticals. Frustratingly, the synthesis of these units appears to be treated on a case-by-case basis.

We have uncovered a general route to this unit using a palladium-mediated carbonylation strategy. This new approach can deliver any diastereomer of the 3-oxygenated tetrahydrofuran unit, and either enantiomer in as little as four steps. We have applied this methodology to the synthesis of antipodal natural products which are not available from natural sources, and are currently using it to access complex natural products.

Ligands for novel transformations (Recsei):

The class of binol derived ligands occupies a privileged position in

the arena of synthetic organic chemistry. Of particular importance in this respect is the subset of ligands based on the 3,3’-disubstituted binol scaffold. With an appropriate choice of sterically demanding substituent at these flanking positions, impressive levels of enantio- and diastereocontrol have been realised over a wide range of transformations. We are interested in utilising 3,3’-dipyridyl substituted binol ligands for organocatalytic applications. As such we have devised a rapid, 3-step synthesis based on the microwave assisted Suzuki coupling of trifluoroboronates. Using this approach, we have synthesised a series of ligands in overall yields ranging from 53 – 100%. This library of ligands will be utilised in a series of organocatalysed transformations.

N-acyl pyrroles (Phippen): The α,β -unsaturated N-acyl pyrrole unit offers many opportunities in the arena of synthetic organic chemistry. We are conducting syntheses that exploit the high electrophilicity of the alkene, the activated nature of the acyl unit and which utilise the masked aldehyde group inherent in the structure. We have recently used this functional group to facilitate the energy efficient synthesis of a key pharmaceutical agent.

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DR CHIARA NETO



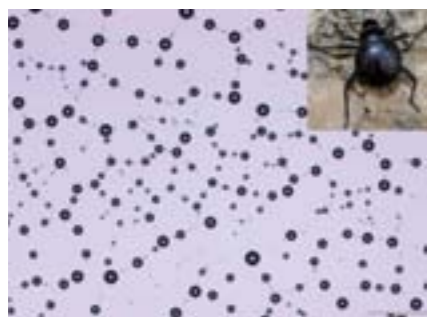
The Neto group 2010

NANO INTERFACES

Our research focuses on investigating the properties of solid/liquid interfaces on the nanoscale, with the aim to design new functional materials. We investigate fundamental physico-chemical mechanisms that have the potential to lead to new technological applications.

Functional Coatings (*Thickett, Harris*): We developed a new chemically and topographically micro-patterned surfaces that can collect water from humid atmosphere. The surfaces are patterned using a spontaneous process, thin liquid film dewetting, which leads to the formation of isolated hydrophilic droplets on a hydrophobic background. The produced patterns mimic the surface structure that is present on a beetle native of the Namib desert, which collects drinking water on its micro-structured back. So far we have achieved collection rates of the order of 10 L/hour/square meter of surface. Future research could lead to the use

Figure 1



of these coatings in the real-world, to provide decentralised and convenient water collection means to solve water shortage problems in our cities (Figure 1).

Biocompatible surfaces through micro-patterning (*Thickett, Telford, Gamble, Meagher*): The ability to control protein and cell positioning on a microscopic scale is crucial in many biomedical applications. We achieved micro-patterning of proteins and cells on surfaces, using self-assembly principles, such as the dewetting of unstable polymer films, followed by selective adsorption of proteins. We can engineer the surfaces so that they are composed of micro-sized protein-adhesive patches in a background that is made protein-repellent by grafting polymer brushes. In collaboration with CSIRO and the Centenary Institute, the micropatterning method is being investigated as a means to improve the biocompatibility of stents.

Microfluidics (*Zhu, Lee, Attard*): A huge hydrodynamic resistance slows down liquid flow in microscopic capillaries and our recent discovery of the occurrence of liquid slip at the solid surface promises to solve this problem, fundamental for more efficient microfluidic devices. We developed a new best practice experimental protocol and a new theoretical algorithm to produce accurate and reproducible data using colloid probe AFM. Using this sensitive technique

we can probe the flow of liquids down to the very last nanometers from the surface, and we have measured slip length of the order of 20-30 nm on flat partially wetting surfaces. We are also investigating the slip properties of soft grafted polymer layers and of gas nanobubbles (Figure 2).

Nanopatterns in Block Copolymer Films (*Lim, Bilek, Kondyurin, Perrier*): Thin films of block copolymers can be used to produce templates for large area patterned surfaces for various nanofabrication applications, such as high-density protein-based biosensors. We investigated the morphology of di-block copolymer thin films, and tested the ability to covalently bond proteins to selected plasma-treated nanopatterned surfaces.

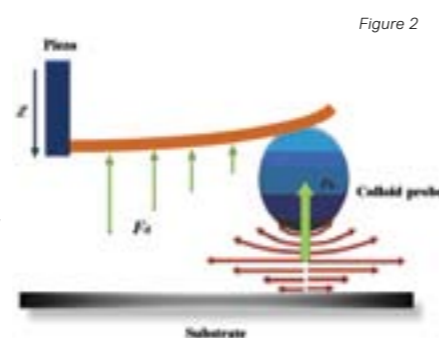


Figure 2

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ORGANIC SYNTHESIS, DRUG DISCOVERY & CHEMICAL BIOLOGY

Our Research is focused on using synthetic organic chemistry to probe problems of biological and medical significance.

Tuberculosis drug discovery (*Cergol, Giltrap, Manos-Turvey, Tran, Britton, West*): *Mycobacterium tuberculosis* (TB), is a devastating human pathogen. Every second a new person is infected with *M. tuberculosis*, resulting in close to 2 million deaths from TB annually. The emergence of multi-drug resistant (MDR) and extensively drug resistant (XDR) strains of *M. tuberculosis* threaten to overcome current drug regimens. TB therapeutics with novel modes of action are therefore urgently needed. We have selected and characterized a number of enzymes from *M. tuberculosis* known to be essential for the growth and survival of the bacterium. This has enabled us to initiate a drug discovery program focused on the design and synthesis of small molecule enzyme inhibitors with a view to discovering new TB drug leads. Representative examples include: 1) The development of inhibitors against salicylate synthase, the first committed step in the biosyn-

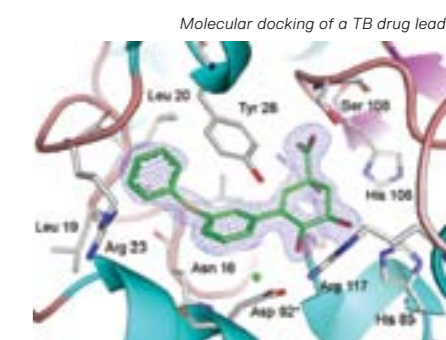
thesis of the iron-chelating siderophore mycobactin T (*ChemMedChem*, **2010**, 1067), 2) Design and synthesis of potent inhibitors of type II dehydroquinase, the third enzyme of the shikimate pathway (*Med. Chem. Commun.* **2010**, 271 and *ChemMedChem*, **2011**, 262) and 3) synthesis of inhibitors of a cell wall lipase based on the fungal-derived natural product tetrahydrolipstatin (*Chem. Commun.* **2011**, 5166).

Marine natural products as antimalarial leads (*Conroy, Hunt*): Malaria is a mosquito-borne infectious disease caused by protozoan parasites of the genus *Plasmodium*, with the most severe human form of malaria caused by *Plasmodium falciparum* (responsible for ca. one million deaths annually). We have developed an efficient chemical synthesis of the natural product symplostatins 4, isolated from the marine cyanobacterium *Symploca* sp. This compound exhibited potent antimalarial activity ($ED_{50} = 40-75$ nM) when tested against the chloroquine sensitive 3D7 strain of *P. falciparum* (*Org. Lett.* **2010**, 5576). This natural product now serves as a lead for the synthesis of a library of analogues for the elucidation of new antimalarial drug leads.

Synthetic glycopeptide cancer vaccines (*Al Shiekha, Ball, Malins, Wilkinson*): The over-expression and aberrant glycosylation of the protein MUC1 in epithelial cancers (including breast, colon, lung, ovarian and pancreatic cancers) leads to the clustered presentation of highly truncated, tumour-associated carbohydrate antigens (TACAs) on the cell surface. Glycopeptides which display multiple copies of these carbohydrates represent valuable targets for the development of cancer vaccines. We

have recently discovered new methods to facilitate the chemical synthesis of a library of self-adjuncting, multi-component glycopeptide cancer vaccine candidates (*Chem. Commun.* **2010**, 6249 and *Angew. Chem. Int. Ed.* **2011**, 1635). Immunization studies in mice models revealed that vaccines provided strong adaptive immunity, eliciting antibodies which selectively recognized the tumour-associated glycopeptide epitopes and now serve as leads for the development of a clinical candidate.

Group news: 2010 saw the arrival of a number of new group members including Lara Malins, Anh Tran and Robert Thompson (PhD students), Dr Katie Cergol and Dr Stephen Butler (postdoctoral research associates) and Dima Al Shiekha, Cameron Ball, and Andrew Giltrap (undergraduate researchers). The group's research was profiled in the RSC publication *Chemistry World*, RACI's *Chemistry in Australia* and was highlighted as the frontispiece of several journals.



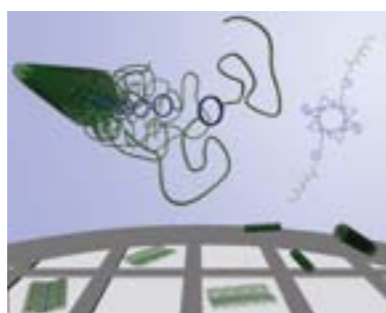
Payne Research Group Christmas 2010



ASSOCIATE PROFESSOR SÉBASTIEN PERRIER

MOLECULAR ENGINEERING

Our research focuses on the synthesis of macromolecules with highly controlled and pre-determinable structures. We exploit supramolecular interactions to organise these molecules into nano-structured materials, for applications in pharmacology (e.g. drug delivery), biology (e.g. antimicrobial materials, synthetic proteins), nanotechnology (e.g. components for optoelectronic applications), material science (e.g. rheology modifiers) or chemistry (polymerisation catalysts, processes, etc.).

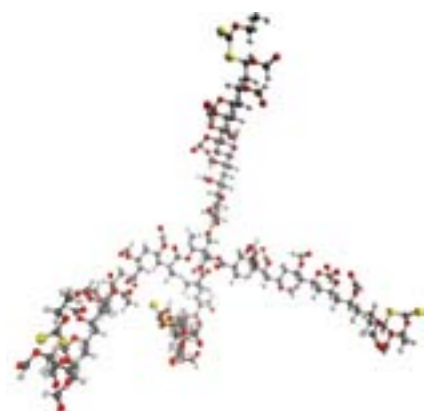


Artistic representation of nanotubes obtained from the self-assembly of cyclic peptide / polymer conjugates

Polymer self-assembly (Chapman, Chun, Dehn, Jolliffe, Kakwere, Lim, Neto, Payne, Siaw, Sriprom): The use of the self-assembly of polymeric structures to design materials at the nanoscale is one of our main fields of interest. In 2010, we developed new synthetic polymers and synthetic polymers / peptide conjugates that can self-assemble into nano-objects in solution. We produced nanoparticles, nanotubes and nanorods with applications ranging from material science to medicine. We also pursued our studies on the self-assembly of block copolymers in thin films, and demonstrated their application to design ultra-fast photochromic materials.

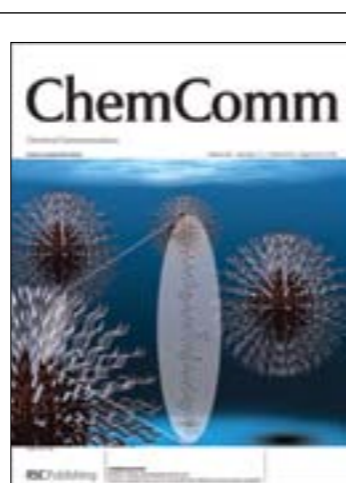
Hybrid synthetic / natural materials (Chapman, Jolliffe, Kakwere, Koh, Maschmeyer, Moraes, Poon, Semsarilar, Tom, Zhao): Combining polymer synthesis to natural polymers enables the design of new materials, which combine the functionality and properties of both natural and synthetic polymers. In 2010, we pursued our work on the use of radical polymerization to control the growth of functional polymeric chains attached to peptides sequences and design functional nanoobjects. We also developed further our pioneering work on conjugation of synthetic polymers to silica (partly in collaboration with the team of Prof Zhao from Soochow University, China) and cellulose, to produce functional and sustainable materials.

Polymer synthesis (Dehn, Hornby, Kakwere, Koh, Konkolewicz, Ladmira, Moraes, Poon, Semsarilar, Siaw, Tom, West): Two of the key polymerisation techniques used in our group are reversible addition fragmentation chain transfer (RAFT) polymerisation and transition metal mediated living radical polymerisation (TMMLRP), which are radical processes that allow the synthesis of complex polymeric architectures in a simple manner. We also investigate high yielding addition reactions (so called 'click' reactions) to modify macromolecules. An important section of our research focuses on the design of new macromolecular architectures via radical polymerization.



A star copolymer

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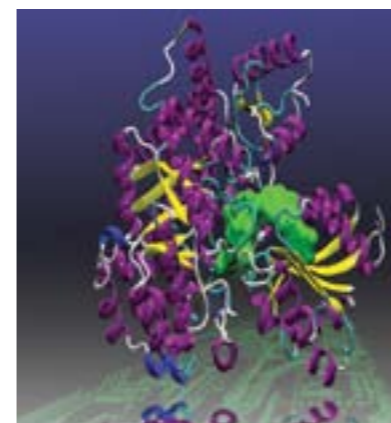
Our article on the self-assembly of polymer / peptide conjugates made the cover of ChemComm.¹

1. Kakwere, H; Chun CKY; Jolliffe, KA; Payne, RJ and Perrier, S. Polymer-peptide chimeras for the multivalent display of immunogenic peptides. *Chem. Commun.*, **46** (13), 2188-2190, 2010.

PROFESSOR LEO RADOM, FAA

COMPUTATIONAL QUANTUM CHEMISTRY

Chemistry is traditionally an experimental science. However, recent advances in computer technology and the development of highly efficient computer algorithms have opened the way for a viable alternative approach to chemistry: chemistry by computer. We use such computer calculations, based on the laws of quantum mechanics, to determine the structures of molecules and to help understand how molecules react with one another.

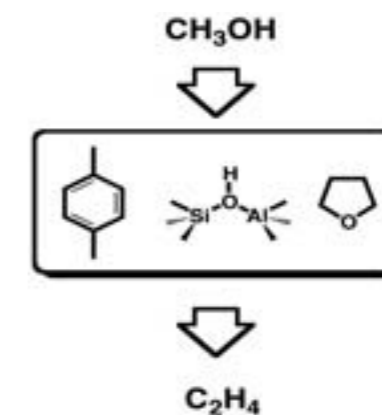


Enzyme-catalysed reactions (Sandala, Bucher, Durbeej, Kovacevic, Baric, Smith): Vitamin B₁₂ is one of nature's essential vitamins. We have used ab initio quantum chemistry calculations to try to understand how coenzyme B₁₂ facilitates certain reactions. We have proposed mechanisms involving partial-proton-transfer (donation or acceptance) provided by enzymatic hydrogen bonding. Supporting evidence for our proposals has come from site-directed mutagenesis experiments. We have reviewed our contributions in this field in a 2010 *Accounts of Chemical Research* article.

Fundamentals of free radical chemistry (Menon, Chan, Taylor, Sandala, O'Reilly, Coote, Henry, Bally): Radicals are ubiquitous in chemistry, biology, and polymer science. Because they are reactive species, they are often difficult to study experimentally and therefore theory has a potentially useful role to play in their characterisation. However, there are also challenges for theory, and the development of new theoretical procedures for treating open-shell systems is an important area of research. We have formulated and tested new procedures, including the G4-SP and G4-sc methods, particularly designed to better describe free radicals.

Peptide radical chemistry (O'Reilly, Chan, Taylor, Jacob, Ivanic, Bacskay, Easton, Davies, O'Hair): An understanding of the oxidation of proteins by free radicals is of great importance because of its implication in a number of human disorders such as Alzheimer's disease, atherosclerosis, and diabetes, as well as aging. We have been using high-level quantum chemistry calculations to address the problem. Specifically, we have been examining the abstraction of hydrogen by chlorine atom in small amino acids and related model systems.

HOCl-mediated damage to proteins (O'Reilly, Karton, Pattison, Davies,



Nagy, Winterbourn): Activated white blood cells secrete the enzyme myeloperoxidase, which catalyzes the reaction of H₂O₂ with Cl⁻ and Br⁻ to produce HOCl and HOBr. HOCl has important antibacterial properties but excessive or misplaced production of HOCl has been implicated in several diseases, including atherosclerosis, inflammatory diseases and some cancers. Both HOCl and HOBr are able to induce N-halogenation of a number of biologically important molecules. We have been investigating the factors that influence the structures and stabilities of the resulting N-haloderivatives, and are attempting to understand the mechanism of their formation. In related work, we have been examining the reaction of peroxiredoxins with H₂O₂.

Hydrogenation and hydrogenolysis (Chan, Amos): We are using theory to try to design systems in which metal-free hydrogenation and hydrogenolysis reactions can occur with low energy requirements. As part of such studies, we have designed a new class of zeolites that show the potential to transform carbon dioxide to methanol at a low energy cost. We have also identified catalysts that can potentially convert methanol to hydrocarbons.

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PROFESSOR JEFFREY REIMERS, FAA

MOLECULAR ELECTRONICS, PHOTOSYNTHESIS

Our work concerns the development of theoretical and computational methods for the prediction and interpretation of the properties of large molecular systems. Quantum-mechanical treatments of electronic and nuclear structure lead to predictions of spectroscopic properties, charge and exciton transport properties, steady-state conductivity, and coherence/decoherence effects.

Photosynthesis and photovoltaics (*Hush, Lee, Crossley*): The conversion of optical to chemical energy by plants is central to most forms of life on this planet. A priori computational methods were developed for predicting the rates of photochemical processes involving charge separation and subsequent recombination in molecules designed for applications in organic photovoltaics. These were used to identify the nature of fundamental processes in ferrocene-porphyrin-fullerene solar-energy conversion molecules. New materials for use in semiconductor dye solar cells were designed and tested. See figure 1.

Molecular electronics (*Chin, Wohlthat, Wang, Hush, Crossley*): Molecular electronics involves understanding the properties of single molecules used as wires to transport electrical current or optical energy, to store information, or to perform other logic tasks. It provides in principle ways of scaling electrical devices beyond

the limits of CMOS and other existing computer technologies. Our work in 2010 focused on the nature of thiol interfaces of gold nanoparticles. These are believed to be controlled by "superatom" rules governing the metallic core. We showed that while such effects influence nanocluster cluster, the critical chemical properties of clusters such as $\text{Au}_{102}(\text{SC}_6\text{H}_4\text{COOH})_{44}$ akin to the shown $\text{Au}_{102}(\text{SCH}_3)_{44}$ cluster shown are controlled instead by local chemical bond strengths. In other work we determined an efficient algorithm for the simulation of the structural and electronic properties of large fragments of graphene. See figure 2.

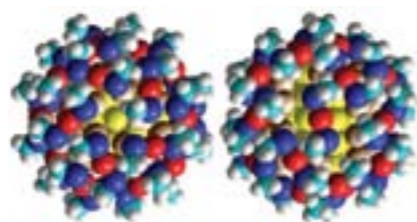


Figure 2

Underpinning fundamental science (*Cai, McKemmish, Flaklof, Hush*): Fundamental research is performed in areas such as molecular conduction and control, solvation, quantum chemistry, and quantum mechanics in order to determine effective means for dealing with both simple and complex chemical systems. In 2010, research focused on the

way chemical reactions occur through transformation of one local-minimum chemical structure to another. This occurs first by nuclear deformation of the reactants, second by an electronic structure rearrangement, and finally by relaxation of the nuclear deformation of the products. This analysis allows many types of chemical reactions and non-adiabatic processes to be viewed from a consistent chemical perspective.

Selected publications

Wohlthat, S; Reimers, JR and Hush, NS. Accurate and computationally efficient third-nearest-neighbor tight-binding model for large graphene fragments *Phys. Rev. B*, **81**, 195125/1-8, 2010. DOI 10.1103/PhysRevB.81.195125

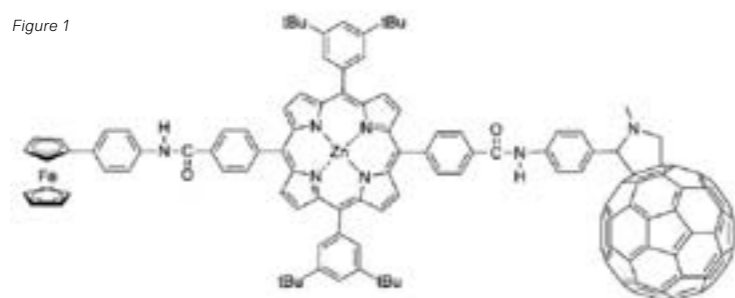
Reimers, JR; Wang, Y; Cankurtaran, BO and Ford, MJ. Chemical analysis of the superatom model for sulfur-stabilized gold nanoparticles. *J. Am. Chem. Soc.*, **132**, 8378-84, 2010. DOI 10.1021/ja101083v

Politzer, P; Reimers, JR; Murray, JS and Toro-Labbe, A. Reaction force and its link to diabatic analysis: A unifying approach to analyzing chemical reactions. *J. Phys. Chem. Lett.*, **1**, 2858-62, 2010. DOI 10.1021/jz101135y

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Figure 1



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Our research group has a strong interest in the development of new agents for an exciting experimental cancer treatment known as Neutron Capture Therapy (NCT), one of the few groups in the world to be involved in this area of research. To date, we have discovered several new classes of DNA- and tumour-targeted compounds and we are currently exploring their potential as NCT agents. Our research is funded by organizations including the Australian Research Council, Cure Cancer Foundation of Australia and The National Breast Cancer Foundation.

Pt-B complexes as new agents for BNCT (*Ching, Clarke, Collins**, *Hosseini, Rutledge*): We have recently explored the preparation of DNA metallointercalators possessing simple boronic acid derivatives, e.g. $[\text{Pt}(\text{trpy})\text{L}](\text{NO}_3)_n$ ($\text{L} = 3\text{- or }4\text{-pyridineboronic acid, } n = 2$; $\text{HL} = 4\text{-mercaptophenylboronic acid, } n = 1$) and $[\{\text{Pt}(\text{trpy})\}_2(\mu\text{-pzB})](\text{NO}_3)_3$ ($\text{HpzB} = 4\text{-pyrazoleboronic acid}$). Selected compounds can bind avidly to sugars such as D-fructose in aqueous solution with $K_{\text{eq}} > 10^5 \text{ M}^{-1}$ in all cases. The thermodynamic parameters of these reactions were determined by using the ITC technique, and preliminary DNA-binding experiments with calf-thymus

DNA showed potent DNA binding for selected complexes. Chiral, boron-rich platinum(II) complexes of the type $[\text{PtL}_2(\text{phen})](\text{NO}_3)_2$ and $[\text{PtL}(\text{trpy})](\text{NO}_3)_2$ (where phen = 1,10-phenanthroline, trpy = 2,2':6',2''-terpyridine, $\text{L} = R\text{- or }S\text{-}1\text{-}(1, X\text{-dicarba-closo-dodecaboranyl})\text{-}4\text{-pyridylmethanol}$; $X = 2, 7, \text{ and } 12$) were prepared and fully characterized. Their interaction with β -cyclodextrin (β -CD) results in the formation of stable, water-soluble host-guest complexes in which each carborane moiety is encapsulated by the cyclic sugar. The complexes also possess a strong, enantioselective affinity for both β -CD and DNA.

Tumour-targeted boronated phosphonium salts as a new class of agents for BNCT (*Ioppolo, Issa, Kassiou, Li, Morrison, Rutledge, Witting†*): We have recently prepared a number of boronated arylphosphonium salts containing either a carborane or boronic acid moiety that have the capacity to selectively target tumour cell mitochondria. Both types of compounds exhibit excellent uptake into human glioma (T98G) cells *in vitro* but the boron-rich carborane derivatives have the capacity to deliver a greater number of boron atoms into these cells. Preliminary flow cytometry and confocal microscopy studies appear to show mitochondrial localisation for selected compounds. We have also recently prepared some PEG analogues of these carborane derivatives which can be radiolabelled with ^{18}F to monitor their uptake and biodistribution in tumour-bearing animals by PET imaging, the results of which are pending.

Gadolinium agents for neutron capture therapy (*Crossley, Fenton, Harris††, Aitken, Morrison, Wang*): One property of Gd that has yet to be exploited in cancer therapy is the remarkable neutron capture cross-section of the non-radioactive and naturally-occurring ^{157}Gd isotope (2.6×10^5 barns). GdNCT is a potentially superior alternative to BNCT as it possesses one major advantage that has not been exploited in the clinic to date. It makes use of the ^{157}Gd isotope with its immense neutron capture cross-section, *the largest of all the naturally-occurring isotopes and 66 times larger than ^{10}B* . The use of DNA-binding agents and mitochondrial agents for the delivery of Gd to tumour cells is without precedent and their potential as GdNCT agents will be explored in this project. Treatment of A549 human lung carcinoma cells with a novel Pt-Gd complex resulted in the selective aggregation of the intact agent within the cell nuclei, as determined by synchrotron XRF imaging. This work represents the first example of Gd delivery to a tumour cell nucleus by a platinum(II) complex. We have also prepared other Pt-Gd derivatives containing a much more robust ligand system than that utilised in our prototype Pt-Gd complex, and the DNA-binding and cell uptake characteristics of the new complexes are currently being determined. Recently, we initiated a study of mitochondrially-targeted compounds containing Gd^{3+} . Towards this end, the DOTA-derivative 1,4,7,10-tetraazacyclododecane-1,4,7-triacetic acid (DO3A) has been appended to a series of triphenylphosphonium moieties to generate a series of bifunctional chelators for Gd^{3+} . Subsequent biological evaluation of these compounds was performed to determine their *in vitro* cytotoxicity as well as their cellular uptake and localisation in human glioma (T98G) cells. The compounds exhibited low to minimal cytotoxicity and good cellular uptake *in vitro*. Cellular localisation profiles in the XRF maps were dispersed but distinct, supporting a mitochondrial uptake mechanism.

*The University of NSW.

†Sydney Medical School, Univ. of Sydney.

††The University of Adelaide.

DR PETER RUTLEDGE

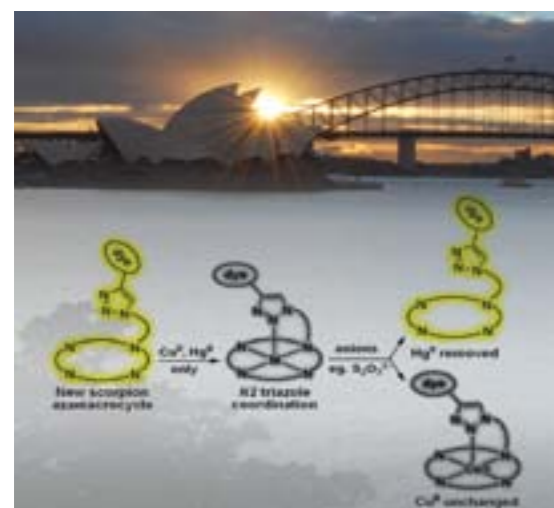
Our research combines organic synthesis with peptide and protein chemistry to develop new drugs and sensors for biomedical applications, biologically-inspired catalysts for important synthetic transformations, and chemical solutions to environmental problems.

BIO-INSPIRED SYNTHESIS AND CHEMICAL BIOLOGY

Metal sensing: In parallel approaches to metal sensing, we have recently reported new fluorescent and electrochemical systems for detecting copper(II) and mercury(II) in solution. A macrocyclic nitrogen ligand and coumarin reporter combine to form a highly responsive, fluorescent sensor for copper(II) and mercury(II) which functions optimally in aqueous solutions at neutral pH (see *Chem. Eur. J.* **17** 2850 (2011), collaboration with Dr Matthew Todd). This azamacrocyclic sensor can even detect copper and/or mercury in doped samples of Darling Harbour seawater (see figure). Work is underway to characterise the mechanism of fluorescence quenching and to extend this methodology to allow the selective detection of other ions in a variety of environmental and biomedical contexts. In a second approach, built on natural strategies for mercury sequestration, we use sulfur-

rich ferrocenyl peptides for mercury detection, characterising metal binding using electrochemistry and NMR. These bio-organometallic compounds respond more strongly to mercury than to other thiophilic metals such as cadmium, silver and lead (see *Tetrahedron* **66** 5653 (2010) and *J. Organomet. Chem.* **696** 715 (2011)).

Hydrocarbon oxidation: The selective oxidation of hydrocarbons to functionalised products (such as epoxides, diols and alcohols) is an important goal in synthesis, but such transformations are often difficult to achieve under mild, environmentally benign conditions. Nature uses iron-based enzymes to catalyse hydroxylation at C–H positions, epoxidation and dihydroxylation reactions. These enzymes use molecular oxygen, the ultimate green oxidant, with water the only by-product. We are developing biocatalytic approaches to alkene epoxidation using a family of non-heme iron(II) enzymes (the soluble di-iron monooxygenases, or SDIMOs) in whole-cell *Mycobacterial* systems (collaboration with Dr Nick Coleman, School of Molecular Biosciences). In a parallel approach, we have created a series of bio-inspired small-molecule iron complexes to oxidise hydrocarbon substrates, and observed iron-promoted alkene dihydroxylation, allylic oxidation and allylic amination reactions (see *Org. Biomol. Chem.* **8** 1666 (2010)).



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Nitrile hydration: The conversion of nitriles to primary amides is another reaction that is difficult to achieve under mild conditions while also being of considerable synthetic interest. Nitrile hydratases execute this transformation in nature, making them interesting targets for biocatalytic and bio-inspired approaches to nitrile hydration. The nitrile hydratase active site contains cobalt(III) or iron(III) bound by two amide nitrogens and three differentially oxidised sulfur atoms. We have built a peptide and peptido-mimetic systems to mimic nitrile hydratase structure and function, characterising these systems using NMR, solution-phase turnover experiments, and XAFS (X-ray absorption experiments in collaboration with Professor Peter Lay and Dr Jade Aitkin).

Antibiotics chemistry: We are also working to characterise the mechanisms of antibiotic biosynthesis (collaboration with Professor Jack Baldwin, Oxford), to devise new mechanisms to combat resistant bacteria, and to develop new antimicrobial agents (see *Org. Biomol. Chem.* **8** 122 (2010), *Biochem. Biophys. Res. Com.* **398** 659 (2010) and *ChemBioChem* **12**, doi 10.1002/cbic.201100149 (2011)).

DR SIEGBERT A SCHMID

INORGANIC SOLID STATE CHEMISTRY AND CHEMISTRY EDUCATION RESEARCH

Research in my group focuses on two major areas. Projects in Inorganic Solid State Chemistry are in general geared towards developing novel and improved materials for use in a range of technological applications. Chemistry Education research projects are designed to improve our understanding of how we best support student learning.

Lead free piezoelectrics (Allen): The fersnoite, $A_2BM_2O_8$ ($A = \text{Ba, Sr}; B = \text{Ti, M} = \text{Si, Ge}$), family of modulated structures has been shown to exhibit excellent piezoelectric properties. Therefore it is one of several alternatives to replace lead-based electroceramic materials.

Variable-temperature X-ray powder diffraction data collected on the powder diffraction beamline at the Australian Synchrotron for a detailed investigation of the structural chemistry of members of the fersnoite-based solid solution $\text{Ba}_{2x}\text{Sr}_{2-2x}\text{TiGe}_y\text{Si}_{2-2y}\text{O}_8$ ($0 \leq x, y \leq 1$) have shown an unusual phase transition on heating for the $\text{Sr}_2\text{TiSi}_2\text{O}_8$ end member composition. This phase transition

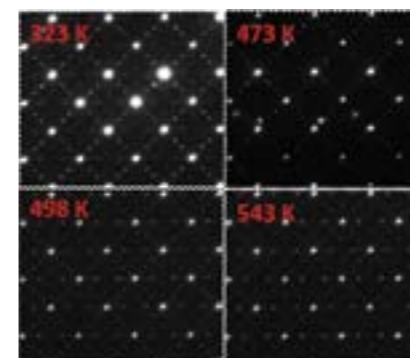


Figure 1: Electron diffraction patterns for $\text{Sr}_2\text{TiSi}_2\text{O}_8$ at 323 K, 473 K, 498 K, and 543 K. The position of the satellite reflections moves from the $[100]^*$ and $[010]^*$ directions to the $[110]^*$ direction on heating, confirming a change from tetragonal to orthorhombic symmetry.

was subsequently studied using the high resolution electron microscope at the Monash Centre for Electron Microscopy (Figure 1). We have been able to show that satellite reflections disappear on heating and reappear on cooling at temperatures consistent with the powder diffraction results. Temperature-dependent changes in cell parameters across the $\text{Ba}_x\text{Sr}_{2-x}\text{TiSi}_2\text{O}_8$ series provide further evidence for a phase transition which removes the modulation from the $\text{Ba}_2\text{TiSi}_2\text{O}_8$ structure at 433 K.

Li-ion batteries (Brant, Kuhn†): Compounds that can reversibly intercalate lithium have the potential to be used as cathodes in rechargeable lithium ion batteries. Two characteristics, the availability of vacant sites for the incorporation of lithium and the presence of reducible cations are found in some defect perovskites. We synthesised a number of defect perovskites, which might be useful as host materials for Li intercalation, and investigated their structures using X-ray and neutron powder diffraction. After careful characterisation of the structures for the Li-free samples, these samples were then chemically intercalated with Li. Subsequently neutron diffraction patterns were collected for two of these samples at RT. It was found that only subtle changes were detectable in the neutron diffraction patterns. Furthermore, the electrochemical intercalation of Li was investigated and in-situ X-ray powder diffraction patterns were recorded during the Li-intercalation process for some samples. We have been able to show that Li-intercalation is possible and best for samples with large vacancy concentrations. In-situ X-ray diffraction showed that the cell dimensions of the investigated samples increased slightly on Li-intercalation, while on de-intercalation they returned to the original value.

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Relaxor ferroelectrics (Whittle): Ferroelectric materials are ubiquitous in technological applications, e.g., from everyday consumer electronics to sophisticated technical instruments. The drive to make smaller and more efficient devices is behind the attempt to develop ferroelectric materials with improved properties. A detailed understanding of structure property relationships is required to develop such materials by design rather than accident. We have investigated four series of compounds in the Ba-Sr-Ti-Nb-O and Sr-Zr-Ti-Nb-O systems which either adopt perovskite, ABO_3 , or closely-related tungsten bronze type, $\text{A}_6\text{B}'_2\text{B}''\text{O}_{30}$, structures. Structural investigations were performed using a combination of synchrotron X-ray and neutron powder diffraction data as well as thermogravimetric analyses. Both composition and temperature dependent phase transitions were established in all systems. A number of our results contradicted some of the sparse information available in the literature prior to the start of this project.

† Collaborators from outside the School of Chemistry

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PROBING MOLECULES WITH LASERS: ASTRONOMY AND SOLAR ENERGY

Our group uses lasers to probe the energy absorption and flow in molecules with applications as diverse as solar energy and astrochemistry

Solar photovoltaic energy presents a tremendous opportunity for society to make the transition to sustainability. However, economic barriers remain to widespread uptake of solar electricity, especially in countries such as Australia, where cheap coal abounds. The imperative is, therefore, to drive down the cost of solar electricity by getting 'more bang for your buck.' Two distinct strategies to achieve this are to make solar cells more efficient or to collect sunlight over a large area and concentrate it onto a much smaller slab covered with solar cells. Both must be achieved at low incremental cost.

Hot carrier cells: As part of an international consortium led by UNSW and funded by the Global Climate and Energy Project, we are developing a hot carrier solar cell to convert in excess of 60% of incoming solar radiation into electrical energy. See: <http://gcep.stanford.edu/research/factsheets/hot-carriersolarcell.html>

Molecular approaches to next-generation photovoltaic-energy conversion (*Crossley, Conibeer, Green (UNSW)*): The flexibility and reproducibility of the optical properties of organic molecules offer opportunities for efficient photovoltaic-device operation. Organic, molecular materials have highly reproducible and controllable optical properties. We are investigating ways in which these attributes may be exploited to increase the efficiency of solar-light harvesting.

We have been investigating triplet-triplet annihilation upconversion (TTA-UC), which uses organic molecules to harvest low-energy light and conjoin the energy of two photons to generate higher-energy radiation. This technique is extremely flexible with regard to wavelength. Using porphyrin molecules synthesized by Max Crossley's research group, we have succeeded in upconverting red to blue (see Figure 1), green, and yellow, as well as green to blue light. Our experiments have shown that TTA-UC can proceed with high efficiency. Kinetic analysis reveals that the process would reach its maximum at a value exceeding 60% (where 100% represents the maximum quantum efficiency of 50%). The kinetic parameters derived from these experiments allow us to evaluate the expected efficiency under solar irradiation. Although this

Figure 1



remains in the few-percent range under sunlight, we anticipate steady improvement as we continue to optimize kinetic parameters. See: <http://spie.org/x42537.xml?ArticleID=x42537>

Luminescent solar concentrators: (LSCs) were proposed in the 1970s as a way to collect a large area of sunlight and direct this onto a small slab of solar cells. Light falls onto a planar waveguide doped with a highly fluorescent material such as an organic dye. Normally, about 75% of the re-emitted light is trapped inside the waveguide by total internal reflection and guided onto the edges of the slab, which are dressed with photovoltaic cells. We have been investigating luminophore alignment, where the fluorescent dye's electronic-transmission moment is held perpendicularly to the waveguide. This results in demonstrated decreases in emission from the top and enhanced emission from the edges of the waveguide as the percentage of trapped radiation increases to 94%.

Laser spectroscopy of hydrocarbon radicals (*Kable, Bacskay, Nauta*): In our gas phase spectroscopy laboratory, 2010, saw the accumulation of spectra of many transient hydrocarbon radicals of potential relevance to fields such as astrochemistry and combustion.

The D_{3h} phenalenyl radical ($C_{13}H_9$) was observed in the gas phase for the first time by both 2-photon 2-colour resonant ionization time-of-flight mass spectrometry, and laser-induced fluorescence spectroscopies. Analysis of its spectrum reveals the interplay between 4 electronic states through both Jahn-Teller and Herzberg-Teller mechanisms. The interesting radical is a test for quantum mechanical theories of molecules, and may prove to be an important interstellar species.

This work was presented at a plenary lecture in conjunction with the receipt of the 2010 Coblentz Award.

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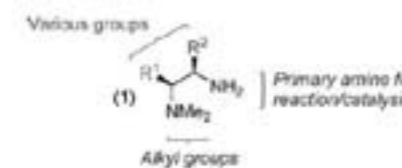


ORGANIC SYNTHESIS, OPEN SCIENCE AND MEDICINAL CHEMISTRY

Our lab motto is: To make the right molecule in the right place at the right time. While figuring out what this means, my students try to make molecules in new ways, observe their interactions with biomolecules and think up ways to solve scientific problems.

New organic reactions

Synthesis is the most enabling part of chemistry, which is itself the most central of sciences. To discover new ways to construct molecules is the lifeblood of our discipline. We have recently discovered several carbon-carbon bond forming processes that generate new chiral diamines (1), a class of compounds that is of central importance to both medicine and asymmetric catalysis. Moreover, my students have found ways of making these reactions asymmetric, providing enantiopure diamines which have previously been inaccessible. The industrial significance of these reactions makes this one of the most exciting and productive new areas for the group's research.



Open science for synthesis and medicinal chemistry

We recently demonstrated an important proof of concept – that a challenging research problem can be solved more quickly if the research is carried out openly and anyone can participate. The problem was the preparation of an important drug for the neglected tropical disease schistosomiasis (Bilharzia). Our collaborators at the World Health Organisation needed this inexpensive drug, praziquantel, as a single enantiomer on a large scale. To make a drug asymmetrically without increasing the price is a problem that industry and academia are ill-equipped to tackle.

Traditionally, science is conducted through a process of pre-publication peer-review originating from papers submitted by groups often working in isolation and in competition with one another. Rather than using this model we reported all of our research openly on the web, and this simple change encouraged a large amount of spontaneous assistance from around the world, resulting in a rapid solution to the synthetic problem which WHO is now scaling up. The chemical industry was a particularly prolific source of both

advice and real experimental support. (A report on the project in Nature may be found at <http://bit.ly/cyWmbV>.)

We are now extending this to the larger, and very exciting, problem of the rest of the drug discovery process. Starting in 2011 we are going to be conducting open source drug discovery for malaria with collaborators at the Medicines for Malaria Venture. All data will be posted online, and there will be no patents. Crucial to the project will be the input of scientists around the world – the Wisdom of the Crowd.

New "magic-bullet" drugs using responsive coordination chemistry

My group pioneered a new kind of coordination compound that changes its shape in a defined way when it binds a biological molecule. The central metal atom of these complexes is coordinated by a "scorpion" ligand that is removed upon binding, and the metal acts as a sensor of this event. We are working with Peter Rutledge's group to adapt this important idea for various medical areas, since such selective responses to biological molecules embody the original concept of magic bullet drugs. We have successfully attached a range of small molecule ligands to these new metal complexes, and are now evaluating their fundamental behaviour in biological media. We were recently awarded a grant to develop the idea into a sensor for breast cancer.



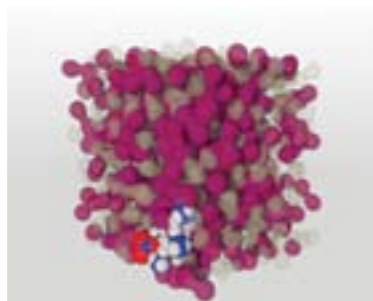
PROFESSOR GREGORY WARR

SOFT CONDENSED MATTER AND INTERFACES

Our research is aimed at understanding nanostructures formed in solutions, lyotropic liquid crystals, complex fluids and in emulsions, foams and dispersions. We pursue a wide range of projects using techniques including neutron and X-ray scattering, optical microscopy, rheology and calorimetry. By combining these techniques we are discovering and designing new nanostructured materials.

Structure and self-assembly in ionic liquids (Zhang, Bernard, Sharma, Atkin,* Hayes*): Our recent work has focused on understanding how the structure and H-bonding between cations and anions affects the structure of room-temperature ionic liquids, and its properties as a solvent. Using neutron diffraction we have revealed that ionic liquids form a bicontinuous network structure by association of short alkyl tails, making them the world's littlest amphiphiles. Changing cation and anion has a strong effect on liquid structure, which can be further modified by dissolving salts into the ionic liquid. This will lead to new understanding of how ionic liquids act in diverse applications including as catalysts and as selective solvents for self-assembled materials and synthesis.

Ionic liquids are also novel media for colloidal dispersions and other multiphase complex fluids. We have formed rigid emulsion gels by dispersing oils into ionic liquid lyotropic phases, and



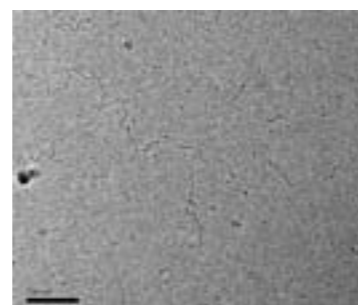
Ionic liquid structure from neutron diffraction shows interpenetration of polar and apolar networks

viscoelastic ionic liquid solutions incorporating worm-like micelles.

Magnetic nanoparticles and ferrofluid (Danos, Zhang, Jain): We investigate how magnetic nanoparticles behave when dispersed in unusual carriers such as ionic liquids and lyotropic mesophases, including a new record stable ferrofluid in an ionic liquid. Magnetic nanoparticles can be inductively heated, so that they can change the state of the fluid in which they are dispersed, causing it to gel or flow, or to change its optical properties.

Polymerisable surfactants (Baptista, Chatjaroenporn, FitzGerald, Baker): We previously showed that the textbook picture of free-radical polymerization of micelles into nanoparticles is incorrect. Rather, polymerisation yields elongated polymer + monomer mixed structures, then collapsed polymeric micelles. These remain in dynamic equilibrium with their environment and their structure can be modified by changing counterion, salt or temperature.

Our new, reactive alkylpyridinium surfmers polymerise in aqueous solution to yield controllable distributions of oligomers. During polymerisation, their structure changes from globular to elongated or even inverted structures as a function of conversion.



Cryo-transmission electron micrograph showing coexisting worm-like and globular micelles

Surfactants with hydrolysable counterions (Liu, FitzGerald): Surfactants with hydrolysable, multivalent counter-ions exhibit several unexpected properties. Small-angle neutron scattering has shown that these surfactants are extremely tenacious in their desire to form spherical micelles. Most remarkable is the ease with which they form phases of close-packed spherical micelles. We have found these in every system studied so far, although previous literature examples are rare.

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Andrew Danos, Connie Liu and Paul FitzGerald scattering x-rays at the Australian Synchrotron



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THEORETICAL MATERIALS CHEMISTRY

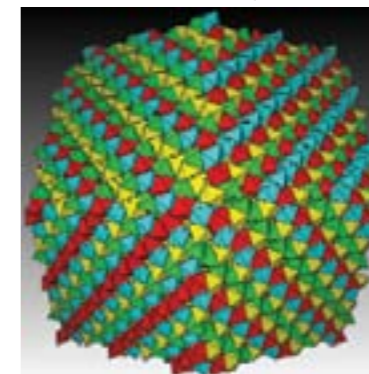
My research focuses on understanding the behavior of complex fluids from a microscopic perspective using the tools of statistical mechanics and computer simulation. The questions I am interested in range from the fundamental to the applied, and often involve the study of beautiful structures that appear spontaneously in systems driven by disorder. To inspire this work and to stimulate research on real physical systems I like to work closely with experimentalists.

Assembly of nanorods for solar energy applications (Baker (Berkeley), Toney (Stanford), Geissler (Berkeley), Alivisatos (Berkeley)): Among the barriers to making cheaper solar cells is the high cost of the single crystalline silicon and vapor deposition methods commonly used today. One possible solution is to print solar cells using an ink of semiconducting nanoparticles. This may also allow for the use of new materials, such as pyrite (fool's gold), and harnessing quantum effects to improve performance. To this end we are using self-assembly to make large 'carpets' of aligned nanorods. This involves understanding how the nanorods interact with one another and with interfaces, how this influences

their phase behavior, and how kinetics affects their aggregation and ordering. At the theoretical level we apply analytical models together with large-scale molecular dynamics and coarse-grained Monte Carlo simulations. By combining insight from theory and experiments we were recently able to report the first cm² films and explain why film formation works better on some substrates. Our paper on this work "Device-scale perpendicular alignment of colloidal nanorods" was among the 20 most downloaded *Nano Letters* in 2010.

Assembly of nano-polyhedra for plasmonic applications (Henzie (Berkeley), Grünwald (Berkeley), Geissler (Berkeley), Yang (Berkeley)): We are working to control the self-assembly of silver nano-polyhedra into 3D supercrystals in order to make materials with possible application in surface enhanced raman spectroscopy, catalysis, and sensing. When light strikes silver it can couple to electron density waves on its surface. By varying the particle shape, their spacing, and how they are packed, we hope to make metamaterials with tunable electromagnetic properties. Recently we demonstrated that it is possible to make highly uniform mm-sized supercrystals consisting of over 10⁸ particles using a relatively simple sedimentation process. We explained the forces that must be balanced to

Figure 1. A new packing of octahedra formed by the self-assembly of silver nanoparticles.

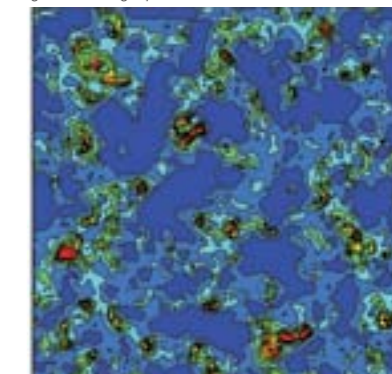


achieve this, and showed that it is possible to make the densest known packings of a wide range of polyhedral shapes including cubes, cubeoctahedra, and octahedra. Finally, we showed that it is possible to change the crystal lattice by introducing polymers into the solution, and discovered an entirely new packing of octahedra with complex helical motifs (Fig. 1).

How do viscous liquids flow?

(Candelier (Saclay), Kummerfeld, Dauchot (Saclay), Biroli (Saclay), Harrowell, Reichman (Columbia)): When a liquid is cooled sufficiently fast, it flows slower and slower until eventually it becomes a solid that lacks long-range crystalline order. This gradual glass transition is at the heart of how optical fibres are formed, super-elastic metals are made, and the rewritable CD functions. Understanding how and why this process occurs, however, is a fundamental problem that has puzzled scientists for over 100 years. We have shown that while glass-forming liquids lack long-range order they nevertheless have long-lived local and medium-range structure that influences their dynamic properties (Fig. 2). Recently we have shown that relaxing atoms are clustered in space and time, forming microscopic avalanches, with strong similarities to experiments on granular materials.

Figure 2. The pattern of structurally soft regions in a glass-forming liquid.



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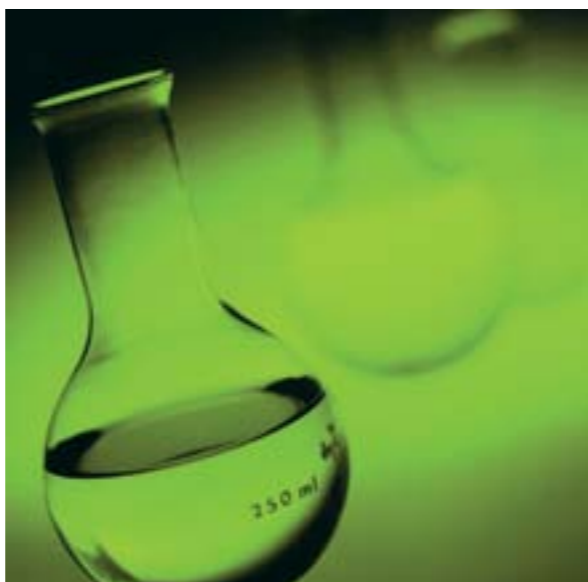
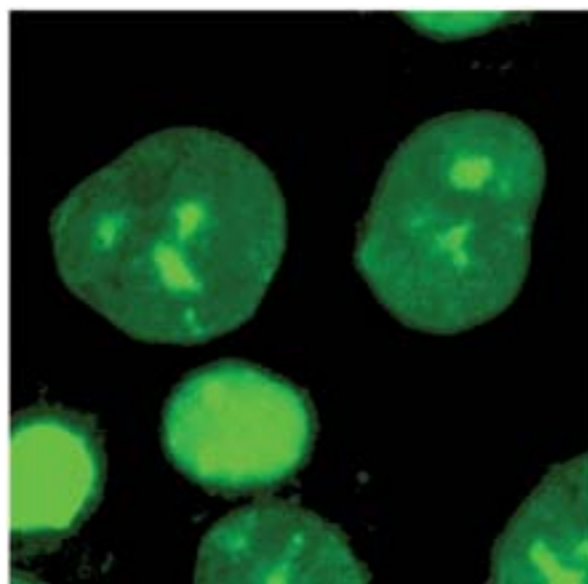
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Dr Julia James, Honorary Associate Professor within the School of Chemistry, emerging after water sampling from Koonalda Cave, Nullarbor Plains, SA.

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The School of Chemistry awards over \$85 000 in Prizes and Scholarships each year to the best of its students. The following students were awarded prizes or scholarships for academic achievements at an awards ceremony in 2011 based on their academic achievements in 2010. Scholarships are awarded subject to the students satisfying conditions required for each of the individual scholarships.

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Awarded to Honours and Postgraduate students for excellence in research in organic chemistry.

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Awarded to the student gaining the combined highest marks in both Semester 1 and Semester 2 Core Intermediate Chemistry unit of study.
Mr Andrew Giltrap

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Awarded for outstanding improvement in Chemistry performance between junior and intermediate Chemistry unit of study.

Mr Alexander Siviour

C.H. Wilson Prize

Awarded to a student graduating in first position with First Class Honours in the area of Organic Chemistry.

Mr Derrick Roberts

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Mr Daochen Tong

Janet Elspeth Crawford Prize in Chemistry

Awarded for the most proficient female student who has completed Chemistry Honours.

Ms Laura McKemmish

Levey Scholarship No. 2

Awarded for proficiency in both Semester 1 and a Semester 2 Junior Chemistry unit of study by a Science, Arts or Engineering student who is proceeding to Intermediate Chemistry.

Ms Zoe Hungerford

Levey Scholarship No. 3

Awarded for proficiency in both Semester 1 and a Semester 2 Junior Chemistry unit of study by a Science, Arts or Engineering student who is proceeding to Intermediate Chemistry.

Mr Malcolm Ramsay

RJW Le Fèvre – DAASN RAO Prize for Physical Chemistry

Awarded for outstanding performance in Physical Chemistry at the Senior Chemistry level.

Mr Jim Gee

Slade Prize

Awarded for proficiency in the practical component of both a Semester 1 and a Semester 2 Intermediate Chemistry unit of study.

Ms Sarah Carman

Walter Burfitt Scholarship No. 1

Awarded for proficiency in both Semester 1 and Semester 2 Senior Chemistry units of study by a student proceeding to Honours in Chemistry.

Mr Jack Orford

R.J.W. Le Fèvre Research Travelling Scholarship

Awarded to an outstanding female postgraduate student to present a paper or poster dealing with her research at a major international conference.

Ms Jessica Chadbourne

Surface Coating Association Australian Scholarship

Mr John Moraes

John A. Lamberton Research Scholarship

Awarded to postgraduate students whose research areas emanate from and are inspired by the work of Dr John A. Lamberton. Thus leading to a greater understanding of the relationships between chemical structure and biological activity.

Ms Corinne Beinat

Mr William Jorgensen

Ms Lara Malins

Mr Christopher Phippen

George Harris Scholarships

This scholarship is awarded annually to students who have completed two years of study towards the degree of Doctor of Philosophy for their contribution to the research and teaching activities in the School.

Ms Lisa Cameron

Mr Stephen Kolman

Ms Caroline Nesbitt



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GRADUATE DIPLOMA IN SCIENCE

The following students had their degrees awarded in 2010:-

Mr Masood Naqshbandi

Development of a re-iterative strategy for the synthesis of polycyclic ethers

Supervisors: Professor John Canning and Professor Maxwell J. Crossley

Mr Yusuf Ziya Sahin

Investigating nanowire growth using block copolymer templates

Supervisor: Dr Chiara Neto

BACHELOR OF SCIENCE (ADVANCED) WITH HONOURS

The following students had their degrees awarded in 2010:-

Ms Natalie M. Baptista

Oligomeric alkylpyridinium surfactants: Novel production and self-assembly behaviour

Supervisor: Professor Gregory Warr

Mr Andrew N. Danos

Amphiphile phase transitions induced by magnetic hyperthermia

Supervisor: Professor Gregory Warr

Mr Jehan Rux Rustom Kanga

New multifunctional porous coordination polymers

Supervisors: Dr Deanna D'Alessandro and Professor Cameron Kepert

Ms Sian L. Myers

Evolution of heat by the Na⁺,K⁺-ATPase: Implications for warm-and cold-blooded species

Supervisor: Dr Ron Clarke

BACHELOR OF SCIENCE (HONOURS)

The following students had their degrees awarded in 2010:-

Mr Duncan Andrews

Non-transition state dynamics and multiple mechanism reactions in the photodissociation of small aldehydes

Supervisors: Dr Meredith Jordan

Mr Stephen Bernard

Bulk and surface structure of metal nitrate ionic liquid mixtures and their ability to support self assembly

Supervisors: Professor Gregory Warr

Ms Marina Cagnes

Synthesis and conformational analysis of α,β,γ -trifluoro- δ -amino acid derivatives

Supervisor: Dr Luke Hunter

Ms Catherine Chen

The influence of structure on the rate of reduction for platinum(IV) complexes

Supervisor: Professor Trevor Hambley

Mr Matthew Terence Dunstan

Studies of hydrated barium oxides: A finely balanced system

Supervisor: Dr Chris Ling

Ms Anna Goldys

Development of a re-iterative strategy for the synthesis of polycyclic ethers

Supervisor: Dr Chris McErlean

Mr Daniel Arthur Hutchinson

Synthesis of tripeptide precursors to cyclobutanone antibiotics

Supervisor: Dr Peter Rutledge

Ms Laura McKemmish

Exploring quantum entanglement and quantum computers through the combined perspectives of computational chemistry and quantum computational physics

Supervisor: Professor Jeffrey Reimers

Mr Michael James Murphy

The design and synthesis of multifunctional coordination frameworks corresponding to NbO-type nets

Supervisor: Professor Cameron Kepert

Ms Teresa Van Nguyen

Chemo-enzymatic approaches to epoxide-derived natural products

Supervisors: Dr Peter Rutledge

Mr Gerard Dean O'Connor

Gas phase spectroscopy of the phenalenyl radical

Supervisor: Associate Professor Tim Schmidt

Mr David Porter

Allylic aminations using iron oxidation catalysts with N-boc-hydroxylamine

Supervisor: Dr Peter Rutledge

Mr Derrick A. Roberts

Singlet oxygen mediated up-conversion of near-infrared light

Supervisors: Professor Max Crossley and Associate Professor Tim Schmidt

Ms Millie Xue

Design, synthesis and biological evaluation of tetrahydropipstatin analogues as tuberculosis drug leads

Supervisor: Dr Richard Payne

Mr David T. Yoo

Structure-affinity relationship studies for the N-arylalkyl-2-azaadamantane class of sigma receptor ligands

Supervisor: Professor Michael Kassiou

BACHELOR OF LIBERAL STUDIES (HONOURS)

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Fluorescent monitoring of iron(III) complexes in solid tumours

Supervisor: Professor Trevor Hambley

Ms Jessica N.G. Stanley

Improving sulfur-resistance of Pt, Ru, and Ni aqueous phase reforming catalysts

Supervisors: Professor Thomas Maschmeyer and Associate Professor Tony Masters

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Structure activity studies of carborane-containing phosphonium salts for boron neutron capture therapy

Supervisor: Associate Professor Lou Rendina

MASTER OF SCIENCE

The following students had their degrees awarded in 2010:-

Dr Candy Chun

Synthesis of cancer-associated glycopeptides and glycoproteins

Supervisor: Dr Richard Payne

DOCTOR OF PHILOSOPHY

The following students had their degrees awarded in 2010:-

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Nanozeolites and delamination - potential solutions to mass transfer limitations

Supervisor: Professor Thomas Maschmeyer

Dr Kaitlin Beare

Synthetic approaches to the DEF ring system of integrinycin

Supervisor: Dr Peter Rutledge

Dr Lance Brooker

A complementary mass spectrometric study of endogenous glucocorticosteroid metabolism for doping control

Supervisor: Dr Adrian George

Dr Stephen Butler

Cyclic peptide scaffolds as selective sensors for biological anions

Supervisor: Professor Kate Jolliffe

Dr Hendra Gunosewoyo

Polycarbocyclic compounds as novel P2X7 receptor ligands

Supervisor: Professor Michael Kassiou

Dr Jill Halliday

Analogues of methyllycaconitine: Synthesis and in vitro evaluation of non-competitive nicotinic acetylcholine receptor antagonists

Supervisor: Dr Chris McErlean

Dr Benjamin Hornby

Synthesis of macromolecular architectures as viscosity modifiers using living radical polymerization

Supervisor: Associate Professor Sebastien Perrier

Dr Varangkana Jitchum

Polymerisation of isoprene via the RAFT process and its applications to the design of nanoparticles

Supervisor: Associate Professor Sebastien Perrier

Dr Hamilton Kakwere

Complex polymeric architectures and nanostructured materials from hydroxylated polymers

Supervisor: Associate Professor Sebastien Perrier

Dr Ravinder Kaur

Metal based anti-inflammatory drugs with high efficacy and low side effects

Supervisor: Professor Peter Lay

Dr Arati Kaza

Novel approaches to the catalytic partial oxidation of cyclohexane and 4-tert-butyltoluene

Supervisor: Professor Thomas Maschmeyer

Dr Amalie Pakchung

Studies of linear and cyclic dihydroxamic acid-based ligands: From nature to synthesis

Supervisor: Dr Rachel Codd

Dr Shiva Prasad

Photocatalytic reduction of NAD-using tin(IV)porphyrins

Supervisor: Associate Professor Tim Schmidt

Dr Steven Rowling

Competing electronic states in formaldehyde dissociation

Supervisor: Professor Scott Kable

Dr Helen Salouros

Studies in the profiling of amphetamine type stimulants

Supervisor: Dr Adrian George

Dr Natasha Sciortino

Multifunctional coordination framework materials: Interplay between spin crossover, structure and host-guest chemistry

Supervisor: Professor Cameron Kepert

Dr Mona Semsarilar

Design of renewable materials: A combination of cellulose, RAFT and supramolecular chemistry

Supervisor: Associate Professor Sebastien Perrier

Dr Neeraj Sharma

Synthesis, structure and properties of some novel transition metal-doped bismuth oxides: From fluoite-type to aurivillus-type

Supervisor: Dr Chris Ling

Dr Wilasinee Sriprom

Light-responsive block copolymer films prepared by RAFT polymerisation

Supervisor: Associate Professor Sebastien Perrier

Dr Danial Stocks

Investigation of design concepts for molecular computing

Supervisor: Professor Max Crossley

Dr Tze Han Sum

Synthesis of novel hybrid steroid-porphyrin conjugates for chemotherapeutic applications

Supervisor: Professor Max Crossley

Dr Tze Jing Sum

Cost effective synthesis of a selective gingivitis inhibitor

Supervisor: Professor Max Crossley

Dr Wlastamon Cody Szczepina

Towards the synthesis of amphidinolide H

Supervisor: Dr Rob Baker

Dr Gordon Thorogood

Structure and properties of metal oxides for use in cation exchange

Supervisor: Professor Brendan Kennedy

Dr James Webb

Porphyrin-based surface architectures and anion sensitive pyromellitimide aggregates

Supervisor: Professor Max Crossley

Dr Benjamin Yap

Rational design, synthesis and biological evaluation of porphyrin-antibiotic adducts targeting porphyromonas gingivalis

Supervisor: Professor Max Crossley

Dr Alexandra Yeung

Research based design of online teaching materials in chemistry

Supervisor: Dr Siegbert Schmid

Dr Ali Youssef

Set in stone: Fluoroalkyl-based protective coatings

Supervisor: Dr Meredith Jordan



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CHEMISTRY



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