Contents

3 Welcome
5 Profiles
41 Publications
55 Benefactors
56 Student prizes and scholarships
59 Staff and students
65 Graduates of 2015
The School of Chemistry at the University of Sydney is one of the main centres for chemical research and education in Australia and has access to a comprehensive range of modern research and teaching facilities.

The School attracts an outstanding cohort of undergraduate students including talented students from all states of Australia. It has a large cohort of both local and international postgraduate research students and offers a vibrant and world class research environment.
2015 saw the School of Chemistry sustain and strengthen its leadership position in research and teaching in Australia and internationally. The School contains 36 independent research groups, with all academic staff supported to be active in their own research direction and to develop into leaders in their fields. Our collective research interests are wide and varied, and the achievements of our research groups, led by academic staff members and described in this report, result from the contribution of all School members towards projects that span the traditional discipline of chemistry and reach beyond it to a diverse range of areas, including new materials, renewable energy and medicine. Collaborations both within and beyond the School serve to strengthen our collective research performance.

Our publication output, competitive research grant success and awards to School members all attest to our continued high level of research performance. In 2015, members of the School received over $5M in new research funding, leading to a total of 21 Discovery Grants, 4 ARC Future Fellows; 6 other Fellowships; 2 DECRAs and 4 Linkage Grants from the Australian Research Council, totaling (with other grants) $11M in competitive research funding. In 2015 the School maintained its strong publication record, collectively producing 8 book chapters and 240 research 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 and many of our research students have been awarded prizes for their presentations at such conferences, reflecting both the excellence of the research they are undertaking and their outstanding ability to present this to an audience. Highlights of the awards to staff and students in 2015 include the RACI Burrows Award to Prof Cameron Kepert; the MedChemComm Emerging Investigator award to Prof Richard Payne; Dr Liz New awarded a Young Tall Poppy; postdoctoral researcher Dr Alice Williamson recognised as one of the top 5 under 40 Science communicators in Australia and the award of the 2015 RACI Pat Rodgers Postgraduate Research prize to PhD student Phil Norcott.

Our research leadership in many 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. This is substantially enhanced by the research infrastructure housed both within the School and the new University-wide core facilities, supported by dedicated high-level professional and technical expertise, including 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. Research is also strongly embedded into our teaching program. In addition to the 96 postgraduate research students in the School in 2015 there were 41 Honours students undertaking year-long, research-intensive training, as well as numerous undergraduate scholars completing Talented Student Program research projects and summer research scholarships. This large cohort of students fosters a strong and vibrant research environment, and, together with our visiting seminar speakers and collaborators, contributes to making the School an exciting place in which to work.

Professor Kate Jolliffe
Head of School
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 tripod 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 (Bacskay):

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)
Our research focuses on the computational inorganic chemistry and education of polyoxometalates, which are a huge and structurally diverse class of compounds with remarkable but poorly understood chemical and physical properties. We are also involved in a number of University and nationally funded projects designed to enhance chemical education and the student experience.

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 build from edge and corner sharing octahedra. The octahedral 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 bioorganic 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 $^1A_g \leftarrow ^1A_u$ band in $[\text{PtCl}_4]^{2-}$ with temperature, modelled using density functional calculations which include spin-orbit coupling.

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.
Professor John Canning

The interdisciplinary Photonics Laboratories (iPL) carry out research in all aspects of photonics, from fundamental material studies to novel devices and applications.

Interdisciplinary Photonics

Self-assembled silica (Cook, Shi, Crossley, Rutledge, Ast, Jamalipour, Gibson - RMIT, McDonagh - UTS): Remarkable structural uniformity within packed self-assembled nanoparticle was observed comparing calculations with AFM, SEM and gas adsorption. This platform, ideal for both telecom-munications and sensing, opens up a realistic approach to fabricating meta-materials. It also allowed the storage of proteins for biological work, obtaining superior performance over sol gel glasses.

More immediately, we proposed and demonstrated the utilisation of magnetic induction heating as practical way of making tuneable devices by integrating iron nano or micro particles. We have extended our pioneering smartphone work (the first to demonstrate emission based detection with a smartphone) to explore novel diagnostics using self-assembled structures.

Laser processing of materials (Cook, Lancry, Poumellec & Brisset - France, Shao – Canada, Chen - USA, Martelli - Brazil, Kristensen - Denmark, Glavind – VESTAS, Denmark, S. Gao - China, Perry & Niewczas – UK, Eparaachchi – USQ): Laser processing was used to tune and pattern surface wetting properties of surfaces and materials. On silica hydrophilicity could be increased below an ablation threshold. Above this threshold we can ingeniously combine optical and plasma interference to create 2D “Birnbaum” patterns to increase hydrophobicity. This method enables a novel preparation and fabrication approach to functionalise surfaces for a range of applications including micro-fluidic laboratories, physical adhesion tapes (popularised by gecko feet), and flow optics.

We continue EC FP7 “eFLAG” consortium & Marie Curie Exchange work with Universite de Paris Sud, demonstrating and elucidating femtosecond laser induced nanopores in periodic nanogratings within 3D volume silica glass. A regime akin to sudden condensation of vapourised and glass of lower Si-O coordination arising from dissociation of O2 in the network was pointed out. Under sudden pressures, tensile in nature, the condensation manifests into a porous network sandwiched between the nano fractures – a pure silica zeosil which is incredibly difficult to generate outside of direct chemical precipitation (such as that thought to occur on Mars). This may be the first time in Earth’s history it has been generated this way because fs lasers can impart energy quickly, faster than the phonon relaxation time. Has it happened naturally anywhere else in the universe? The orientation of the nano fractures allows for novel linear and circular birefringence to be arbitrarily introduced and oriented by controlling the laser polarisation. Given 3D spatial control, this allows the potential for unprecedented complex structures within materials.

UK colleagues focussed on a novel industrial application where the packaging of conventional gratings can be perfected through high T induction processes optimised using regeneration to allow measurements to 1400C. We also showed tuning components into high T complex structures, including chirped gratings, exploiting the silica viscoelastic regime and demonstrated an accurate measurement of viscosity of silica in optical fibre form for the first time. And the highest T performing all-contained fibre laser to date was demonstrated with US colleagues. Working with USQ CoE for Composites, new genetic algorithms to resolve sensing data from complex strain profile measurements using chirped gratings were tested.

Optical fibre fabrication (Cook, Peng - UNSW, Luo - UNSW, Shao - Carlton, Kristensen - Aarhus, Glavind – VESTAS, nine partner institutions): A new generation of Bi and Er3+ doped silica fibres allowed single diode pumping to generate an extended ultra-broadband telecom emission. Industrial PhD student from Vestas and Aarhus University has completed his PhD work exploring novel long period gratings within D-shaped fibre fabricated at the national Fibre Facility for sensing strain in the next generation of windmill blades (>80 m in length). What better way than to show how fundamental material studies have progressed to allow fruition of advanced sensing technologies for environmental sustainability.
of molecular hydrogen leading to
dissociative adsorption. This is because
the dissociative H\textsubscript{2} adsorption barrier
on graphite (graphene surface) is
rather prohibitive, approximately 3.3
eV. However dissociation has been
predicted to occur in particular case;
if H\textsubscript{2} approaches a vacancy defect
or edges on a graphene surface, the
molecule becomes largely polarised,
the energy barrier is reduced, and may
finally disassociate.

Dr Mohammad Choucair
The next generation of advanced carbon materials will
need to be synthesised on-demand to address challenges
relating to human health, the environment, and reliable
energy storage.

Materials Chemistry
Novel synthesis pathways to carbon nanostructures
In order to facilitate the widespread use and application of carbon
nanomaterials there is a need for simple, scalable, and feasible processes
to synthesise them. We explore bottom-up chemical pathways to
carbon in a uniform atomistic fashion. In particular, addressing the concept
of ‘hierarchical’ reactions at the surface of formed carbon nanostructures
as these reactions may not obey a single mechanism. A large number
of processes may occur, which are characterised by different relaxation
times; long-lived states including defects and dislocations, and layer
formation which have been directly observed in our non-equilibrium carbon
systems. Many of the reductions to precipitate carbon in different forms
involve controlled thermochemical and mechanochemical reactions, and
characterising the materials using electron microscopy, photoelectron
spectroscopy, and electron diffraction.

Hybrid graphene nanomaterials
The scalable design and synthesis of advanced graphene materials is
necessary to permit sustainable energy use. We are establishing multi-step
synthesis routes to functional graphene architectures that provide access
to high surface areas and energies required for gas storage applications.
The exceptional physical properties of graphene is being combined with
the unique chemistry of transition metal hydride complexes to create
metal-inorganic functionalised hybrid materials. A full complement of
techniques are used to investigate the importance of surface functionality
on the uptake of various gases of the materials synthesised, including:
electron microscopy, infra-red and Raman spectroscopy, nuclear
magnetic resonance, inelastic neutron scattering, and adsorption-desorption
measurements.

Hydrogen adsorption on graphene
Chemically synthesised graphene sheets provide a model system, which
represent both locally high quality graphene and disorder over large scales.
Studies of the interaction between hydrogen and graphene are of interest
due to the potential to chemically modulate the electronic structure of
graphene for device applications and the prospect of using graphene as a
hydrogen storage material.

Our recent collaborative work on the interaction of muons with chemically
produced graphene evidenced that muons (hydrogen analogues) are
mobile on the graphene surface, moving around to find efficient
trapping sites. We know our graphene material may contain defects and edge
sites suitable for trapping hydrogen; electron spin resonance studies clearly
identified itinerant and localised electrons below 50 K. However, it is
still unclear whether vacancy defects in graphene can promote the mobility
of molecular hydrogen leading to
dissociative adsorption. This is because
the dissociative H\textsubscript{2} adsorption barrier
on graphite (graphene surface) is
rather prohibitive, approximately 3.3
eV. However dissociation has been
predicted to occur in particular cases;
if H\textsubscript{2} approaches a vacancy defect
or edges on a graphene surface, the
molecule becomes largely polarised,
the energy barrier is reduced, and may
finally disassociate.
BIOPHYSICAL CHEMISTRY OF MEMBRANES

Mechanism and regulation of the Na⁺,K⁺-ATPase (Cornelius1, Allen2, Rasmussen3): 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 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 of the enzyme to be resolved on the millisecond timescale, isothermal titration calorimetry, which can resolve the heat released in individual reactions, and whole-cell patch clamp, which enables the electrical current across the cell membrane produced by the Na⁺,K⁺-ATPase in a living cell to be directly measured.

In other experiments and molecular dynamics simulations, carried out in collaboration with Professor Toby Allen, we found evidence that the Na⁺,K⁺-ATPase undergoes fluctuations in its membrane hydrophobic thickness in the course of its catalytic cycle. To prevent unsustainable energy losses the surrounding lipid membrane must accommodate these fluctuations by local membrane deformations (see figure).

Role of cholesterol in membrane function: Cholesterol has a very bad reputation. Even amongst the general public it is now common knowledge that high blood cholesterol levels are an important risk factor for the development of cardiovascular disease. Indeed, cholesterol has such a bad name that food companies even use the label “no cholesterol” as a marketing ploy on olive oil, sugar and many other products which have no reason to contain cholesterol at all. However, cholesterol is present in animal plasma membranes to a level of approximately 40 mol%, and animals even synthesize cholesterol via multi-step enzymatic pathways. Therefore, animals must produce cholesterol for some good reason. The aim of this project is to discover the role that cholesterol plays in cell membrane function, a question that has puzzled physiologists, biochemists and biophysicists for decades. In a recent bioinformatics study we found evidence suggesting that cholesterol co-evolved within animal cell membranes to optimise the activity of the Na⁺,K⁺-ATPase and allow the development of multicellularity. We are now undertaking a detailed study on the effects of cholesterol and its derivatives on membrane physical properties to see if these correlate with their effects on membrane protein function.

1 University of Aarhus, Denmark
2 RMIT University, Melbourne
3 Royal North Shore Hospital, Sydney

The focus of our research is on the function of ion-transporting membrane proteins, without which no cellular life forms are imaginable. We are interested in the mechanisms of these enzymes, their physiological regulation by their membrane environment and their chemical evolution. Our major object of investigation has for many years been the sodium pump.
PROFESSOR MAXWELL J CROSSLEY, FAA, FRSN

Novel porphyrin systems were synthesized and used for the study of artificial photosynthesis and as photo-induced water splitting catalysts. Integration of organic substances into self-assembled silica-based materials was achieved.

between adsorption configuration and molecular conformation was elucidated. New ways of stabilizing porphyrin self-assembled monolayers were explored. New synthetic routes to 5,10,15,20-tetra(ω-functionalised-alkyl) porphyrins were established. A priori calculations of the free energy of forma- tion from solution of polymorphic self-assembled monolayers was achieved for the first time. These are shown to predict and/or interpret newly measured and existing high-resolution scanning tunnelling microscopy (STM) images of SAM structure, rationalizing polymorph formation conditions. A wide range of new molecular condensed-matter prop- erties at room temperature now appear suitable for prediction and analysis using electronic-structure calculations.

Synthesis and photophysics of models for the photosynthetic reaction centre (Naqshbandi, Canning, Sintic, Reimers, Fukuzumi,* Ohkubo,* Yamada*): Tris- and tetrakis-porphyrin chemical mimics of the chromophore arrangement of the photosynthetic reaction centre (PRC) have been further studied. These are the closest synthetic mimics of the natural systems to have been developed anywhere. A composite of nearly mono-dispersed Al-containing SiO$_2$ nanoparticles and an organic photocatalyst (2-phenyl-4-(1-naphthyl)quinolinium ion) acts as an efficient catalyst for photocatalytic H$_2$ evolution in water.

Efficient photochemical up-conversion by triplet-triplet annihilation using porphyrins and related compounds (Visser, Schmidt,* Cheng*): Molecular approaches to next-generation photovoltaic-energy conversion are under investigation. Ring annulated porphyrins behave as π-expanded systems and they are very efficient sensitizers for energy upconversion whereby a stream of light of a given photon energy is converted into one of a higher energy. Work continued on the development of phthalocyanine analogues. Synthetic routes to π-expanded phthalocyanine systems were explored but these com- pounds were found to be more difficult to synthesise and be less amenable to scale-up than the previously developed porphyrin compounds.

Porphyrin analogues as Gingivitis inhibitors (Hunter,* Dingsdag*): A series of lysine-linked porphyrin-metronidazole analogues, synthesized in earlier work, are recognized by cell surface HA2 receptors of the gingipains of Porphyromonas gingivalis with very high selectivity. These hybrid compounds were found to be very good inhibitors of the organism. Most importantly, unlike metronidazole, the new inhibitors did not kill a range of other anaerobic bacteria isolated from the oral cavity and human gut. Trans-cell membrane transport and in-cell processing were further studied. The surface lysine-specific gingipain protease that recognises the porphyrin sys- tem was established to not be involved in direct trans-cell membrane transport but is probably responsible for haem μ-oxo dimer production from haemoglobin and its cell-surface accumulation.

Porphyrin bioconjugates (Taba, Sintic): Synthetic and biological studies of porphyrin-steroids based on the natural steroids estrone, estrogen and lithocho- lic acid were completed.
FUNCTIONAL INORGANIC MATERIALS

Light-activated metal-organic frameworks (MOFs) (Healey, Liang): Our work has involved the use of light to modulate the size and polarity of the pores in MOFs by exploiting light responsive photoreduction reactions. We have synthesised novel viologen- and spiropyran-based ligands that have been incorporated into 2- and 3-dimensional materials (Figure 1). The physical properties of these materials have been found to change upon light irradiation. Our ultimate goal is the use of sunlight as a clean and renewable energy source to facilitate gas separations using porous materials.

Radical MOFs and porous organic polymers (POPs) (Usov, Hua): Our work has involved the design and synthesis of MOFs and POPs which exhibit the highly sought-after property of redox activity and ultimately, electronic conductivity. We have developed frameworks based on novel triarylamine radical ligands, as well as ruthenium-based frameworks. Solid-state electrochemistry and novel spectroelectrochemical techniques have been developed to investigate the charge transfer and conductivity properties. The opportunities for advances at a fundamental and applied level are immense, with potential applications ranging from sensors to molecular electronics devices.

The interplay between conductivity and magnetism in microporous materials (Walwyn, Doheny, Kepert): In collaboration with Professor Cameron Kepert, we have synthesised novel triselenafulvalene ligands and have incorporated these into new charge transfer framework structures (Figure 2). Using conductivity, magnetism and EPR studies we are beginning to unravel the origins of unusual physical phenomena which arise from the interplay between multiple framework properties.

Carbon dioxide capture and conversion (Das, Liang, Hua, Solomon, Church, Kepert): The development of more efficient processes for CO\textsubscript{2} capture is considered key to the reduction of greenhouse gas emissions implicated in global warming. Our work has involved the synthesis of novel salen and sulfone-tagged ligands and their incorporation into air- and water-stable MOF and POP architectures. These materials exhibit high selectivities for the uptake of carbon dioxide over the other major components of flue gas streams, and we are currently investigating the nature of the CO\textsubscript{2}-framework interactions which give rise to this activity.

We are also investigating the electro- and photo-catalytic conversion of CO\textsubscript{2} into carbon monoxide and formic acid using novel MOFs and POPs incorporating rhenium and ruthenium metalloligands. This work forms part of a major collaborative project with 18 partners across Australia (supported by the Science & Industry Endowment Fund (SIEF)) to capture and convert harmful greenhouse gases such as CO\textsubscript{2} into useful commodity chemicals.

Figure 1: Schematic diagram of MOF-808 incorporating grafted spiropyran ligands. UV light irradiation induces switching to the merocyanine form which has a higher affinity for uptake of CO\textsubscript{2}.

Figure 2: The novel conducting charge transfer salt TSTF-TCNQ constructed from the new electroactive ligand triselenafulvalene. Conductivity profile and crystal structures down the a (a) and b axes (b).
SYNTHESIS AND ANALYSIS

Detection of drug use in sport (Tangvisethpat): Performance enhancing drug abuse is a persistent problem in the sporting community, as well as in wider society. The need for fast, cheap, broad-coverage screening methods is imperative to ensure fairness in competition and to preserve the health of athletes. Routine testing of athletes in competitive sport involves collection of urine samples. This is a non-invasive form of sampling and provides an inherently sensitive matrix. However, urine may be subject to tampering, has storage and transportation problems and, if the athlete is dehydrated after strenuous exercise, may be difficult to collect. Current blood analyses require invasive venipuncture and relatively large sample volume collection. Improvements in instrument sensitivity have made it possible to explore dried blood spot analyses.

Blood is collected using a ‘finger prick’ method, commonly used to test blood sugar levels. The blood is collected onto a sampling medium (an example is illustrated) which can then be punched out and analysed in the laboratory. This research has coupled High Performance Liquid Chromatography with High Resolution Mass Spectrometry. A fast throughput screening method has been developed as part of the method validation. A total of 230 different drugs in eight classes (anabolic agents, ß2-agonists, hormones, diuretics, stimulants, narcotics, cannabinoids, ß-blockers) have been examined and most can be detected in the low ng/mL range.

Profiling of synthetic illicit drugs (Grzechnik): 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 this has been extended to the optical profiling of methylamphetamine which can indicate the likely starting materials used in the clandestine synthesis of this drug.

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.
RESEARCH PROFILES

MEDICINAL INORGANIC CHEMISTRY
Monitoring the penetration and effectiveness of anticancer drugs in solid tumours (Akerfeldt, Bryce*, Kim): 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 (spheroids) for use as model systems to study anti-cancer drug penetration and the effect of those drugs on cell status and viability. Our group has previously developed a 4-dimensional cellular model of a solid tumour that expresses a photo-convertible green fluorescent protein when the cells are under conditions of hypoxic stress. This model was used to study the response of spheroids to anticancer agents designed to be activated in hypoxic conditions. Development of additional models that report cellular, iron status and cell cycle status continued during the past year. In conjunction with these, spectroscopic imaging and mapping methods, including X-ray fluorescence mapping, were employed to chemically and biologically characterise tumour cell spheroids and to investigate the induced biochemical responses of the tumour model to treatment.

Targeted delivery of metal complexes for anticancer applications (Akerfeldt, Chen, Glenister, Gui, Horry, Klein, Lo, Oxman, Rentrew, Simone*, Tondl, Ze): The preparation of complexes designed to target tumour cells and to improve uptake and activity in the various microenvironments found in solid tumours was continued. These complexes are designed to exploit one or more of: the lower oxygen concentration, the lower extracellular pH, the higher expression of cell membrane bound systems for the uptake of glucose, folate, or PSMA substrates, or the higher extracellular expression of proteases such as matrix metalloproteases and kallikrein 3 (PSA). Studies of cellular and spheroid accumulation and distribution were undertaken for a series of platinum(IV) complexes.

Work was continued into the stabilisation of platinum(IV) compounds and their functionalisation with targeting groups. New examples of a novel series of platinum(IV) complex that generates a positively charged platinum(II) complex on reduction were sought and synthetic strategies for adding targeting groups such as the PSMA substrate were investigated. The intracellular accumulation and reduction of platinum(IV) complexes was studied using XANES. Work was continued on the attachment of sugar groups to the axial sites of platinum(IV) complexes and to the carrier ligands of hypoxia selective cobalt(III) chaperone complexes. New strategies for preparing and functionalising the carrier ligands of the cobalt(III) complexes were developed and cobalt complexes were prepared with novel anticancer agents attached.

PROFESSOR TREVOR W HAMBLEY*

The projects listed below are all associated with biologically active metal complexes. The emphasis is on anti-cancer drugs and our aim is to develop drugs that have a high selectivity for tumours based on their chemistry and biochemistry and have an ability to penetrate into solid tumours. High selectivity will overcome many of the toxic side effects of existing drugs and allow higher doses to be used. Better penetration will enable the destruction of cells that presently evade treatment and contribute to resistance.
THEORETICAL CHEMISTRY
The formation of tubular crystals in atomic alloys (Douglass, Hudson): The spontaneous self assembly of order is fundamental to materials science and molecular biology. The formation of layers and tubes has, up till now, only been observed in complex molecular solutions. In simulation studies we have discovered elaborate tubular crystals in atomic mixtures and showed how they arise from a large size difference that allows for double occupancy of nearest neighbour attractions.

Theory of the interface-mediated shear melting of a crystal (Ramsay): The freezing point of a sheared liquid is depressed by an amount larger than can be explained by the straining of the crystal. We have developed a theory that describes how the erosion of the crystal surface by the flowing liquid can account for the dependence of the melting point on the shear stress.

Long range stress correlations in a fluid at rest (Chowdhury, Abraham, Hudson): A distinguishing feature of liquids and solids is that the latter can sustain long range stress correlations while the former cannot. In this simulation study we showed that the liquid, in fact, does exhibit transient long range stress correlations and that these correlations make an important contribution to the stress fluctuations that determine the shear viscosity of the liquid.

From liquid structure to configurational entropy (Ronceray (Ecole Normale)): The geometrical structure of a liquid consists of a complex arrangement of a variety of local coordination polyhedral. How to understand the physical significance of such structures is an outstanding problem. We have established a formal theory for the configuration entropy of the liquid in terms of the structure, thus allowing us to assess how specific structures contribute to the stability of the liquid state.

The origin of rigidity in configurational constraint (Saw, Abraham): Rigidity defines solids and yet it is not an equilibrium property of materials. In this study we show that the shear modulus of a material is determined by the constraint that is imposed on the averaging over the space of particle configurations, irrespective of how that constraint is imposed.

I am interested in understanding the structure, dynamics and phase transitions of liquids and solids. Topics include understanding the relation between glassy solids and viscous liquids, the factors that control how fast a liquid can freeze and how rigidity comes to be. My tools are model building, computer simulation and theoretical analysis.
POLYMER AND COMPOSITE COLLOIDS

Key functional additives in paint technology (Neto, Nguyen, Zhu, Davey, Baker, Such): The application of controlled radical polymerisation allows a degree of control over polymer and nanoparticle architectures that was previously only dreamt of. From the controlled radical techniques currently available, reversible addition fragmentation chain transfer (RAFT) has proven to be the most versatile. In this broad-based project, funded by DuluxGroup Australia and the ARC, we exploit this new capability to design and synthesise polymer and composite nanoparticles with particular emphasis on applications in surface coatings. Our achievements in this project include coating individual unaggregated pigment particles with polymer (Figure 1) for improved pigment efficiency, reducing the coating amount required. Coating particles in this way has been a “Holy Grail” in the coatings industry for many decades. Pigment efficiency has been further improved by encapsulating individual pigment particles within hollow polymer particles, thus halving the amount of TiO₂ needed to achieve a given opacity. We have also developed a new approach to make Janus particles that is economical and enables large-scale production.

Polymer stabilisation of superparamagnetic nanoparticles for biomedical applications (B. Pham, N. Pham, Kim, Sabouri, Raviraj, Painter, Rozeleur, Tanudji, Jones): In this project, we have designed a steric stabilisation system for nanoparticles in collaboration with Sirtex Medical Limited, and are exploring their use in a wide range of biomedical applications. Such applications include stem cell tracking, treatment of ovarian and colon cancers, and the enhancement of radiation in the treatment of cancer. These particles offer many advantages including easy functionalisation, and are stable in biological media and within cells i.e. they do not aggregate. The particles have been shown to penetrate spheroid solid tumour models, and facilitate the penetration of co-administered chemotherapy drugs. When the core particles used are superparamagnetic iron oxide, they possess excellent imaging properties, with T2 relaxivities of close to 1,000 s⁻¹ mM⁻¹ obtained. We have also used these sterically stabilised nanoparticles to form composite 35 micron beads for the hyperthermia treatment of liver cancer. The beads prepared generated heat at a rate of 20 W/cc.

Controlling density, viscosity and crystallisation in emulsion explosives to enhance safety and efficiency of blasting operations (Warr, Priyananda, Fitzgerald, Djerdjev, Gore): In this collaboration, funded by Dyno Nobel Asia Pacific and the ARC, we are gaining a fundamental understanding that will allow us to control the density, viscosity, and crystallisation in explosive emulsions.

Enhancing the efficacy and performance of agrochemical actives (Huynh, Nguyen, Burns, Schoetz, Heming): In this collaboration with Syngenta Crop Protection, we are using controlled radical polymerisation techniques to assist in the design of safer and more effective delivery systems for agrochemicals.

Ionic liquid ferrofluids (ILFFs) for space propulsion (King, de la Mora, Sabour, Priyananda, Rozeleur, Jones): In this project, funded by AOARD and Sirtex Technology, in collaboration with the US Air Force, Brad King from Michigan Tech, and Juan de la Mora from Yale, we are exploring the use of ILFFs (Figure 2) in the trajectory control of mini satellites.

ASSOCIATE PROFESSOR BRIAN HAWKETT

Our research focus aims to gain an understanding of the factors governing the formation and stabilisation of colloidal dispersions in order to solve the scientific problems that are of interest to our industry collaborators.
THEORETICAL MATERIALS CHEMISTRY

Structural search (Kolli, Tracey, O’Toole, Harrowell): Packing models are often employed to predict and rationalize the architecture of metamaterials, self-assembled from nanoparticles, or colloidal crystals. We have developed a systematic search methodology to find ground state crystal structures for particle assemblies, by enumerating subspaces of the general search space. We have identified a number of new optimal structures in systems of binary spheres, asymmetric dimers, helices, and a general class of 2d shapes. Outcomes include: an explanation for the observed size ratio of silica spheres in a class of precious opals; a simplified understanding of colloidal and atomic alloys which take the NaZn$_{13}$ structure type; and, the first predictions of thermodynamically accessible compound colloidal crystals for binary spheres with large size ratios.

The screw-like nematic phase (Kolli): Helical particles are a key system to understand given the ubiquity of DNA. The phase behaviour of helical strands was presumed similar to that of most liquid crystals, which form in most systems of elongated particles. We recently showed that helices have an additional chiral nematic liquid crystal phase in between the regular nematic phase (aligning) and the smectic phase (layering). Our simulations showed that the orientation of the secondary axis of the helices becomes periodically coupled with translation along its primary axis. We have now also shown that this kind of coupling transition occurs again in high density smectic phases (Fig. 1).

Janus dumbbells (O’Toole): Spherical Janus (two-faced) particles have unusual collective behaviour, including re-entrant behaviour when phase-separated gas-liquids can remix as the temperature is reduced. We are investigating the effect of particle geometry on this behaviour, studying Janus dumbbells. We have found cases where the anomalous behaviour is pre-empted by the formation of lamellar structures. We are currently investigating the trends as the asymmetry of the particle is varied.

Packing efficiency (Jennings, Tracey): What is the relationship between the shape of a particle and its ability to pack densely? This question is still wide open, but work on 2-d shapes in our group has put forward the first phenomenological answer (Fig. 2). Measuring certain properties of a shape, we can accurately predict packing densities. We can start to explain the ubiquitous observation that when molecules crystallize, some crystal symmetries are disproportionately favoured. Why are rotated particle pairs so common?

Amorphous relaxation (Douglass, Chowdhury, Harrowell): 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. These complex events cannot easily be directly probed, because in glasses all we can usually get are averages and distributions. Instead we use models of atomic interactions in network glasses, and glassy binary mixtures of soft spheres. We study both crystallization phenomena and stress relaxation. Stress relaxation is related to the viscosity of a material, and therefore is a key player in the transition from liquid to glassy behaviour (Fig. 3).
Our research focuses on using and developing the tools of organic synthesis for the preparation of molecules with a particular function. Specific targets include molecules capable of recognizing and sensing other molecules, and self-assembling peptide-polymer conjugates.

**ORGANIC SYNTHESIS AND SUPRAMOLECULAR CHEMISTRY**

**Novel anion receptors and transporters** (Yuen, Elmes, Qin, Smith, Tzioumis, Zwicker, Gale*): 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. Similarly, the ability to sense and/or sequester ions such as nitrate and sulfate in aqueous media has applications in environmental science. 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 preorganisation 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. Linear and cyclic peptide derivatives and peptidomimetics that exhibit high selectivity for sulfate ions in aqueous media have also been developed and in collaboration with Prof Phil Gale (University of Southampton, UK) we have shown that some of these can transport sulfate ions across a bilayer membrane.

**Efficient synthesis of natural and novel cyclic peptides** (Taleski): 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. We are employing our previously developed method for the efficient head-to-tail synthesis of small cyclic peptides to the synthesis of cyclic peptides with potential as therapeutic agents in the area of cardiovascular disease and as antibiotics.

**Self-assembling peptide polymer nanotubes** (Long, Warr, Perrier*): In collaboration with Professor Sebastien Perrier (University of Warwick, UK), we are using cyclic peptides that are designed to self-assemble into beta-sheet structures to guide the formation of nanotubes from cyclic peptide–polymer conjugates. The polymeric corona of the tubes can be used to control the length and solubility of the nanotubular structures, thereby providing well-defined polymer-coated nanotubes with a range of applications from materials science to medicine.
INTERMOLECULAR INTERACTIONS

Potential energy surfaces: 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 \textit{ab initio} quantum chemical calculations. These are contained in our freely available \textit{Grow} computer package.

Hydrogen storage materials (Kolmann, D’Arcy): We have used \textit{Grow} to develop a reduced-dimensional model to mimic \textit{H}_2 adsorption in Lithium-doped metallo-organic framework materials such as MOF-5.

Quantum diffusion Monte Carlo (QDMC) simulations have been used to predict \textit{H}_2 binding enthalpies and vibrationally averaged (ground state) structures. They demonstrate that the \textit{H}_2 molecule is delocalised over the organic fragment. We are currently investigating how the quantum nature of such systems changes with temperature and number of adsorbed \textit{H}_2 molecules.

Molecular property surfaces (Morris): Our interpolation techniques have been used to describe molecular dipole moment and polarizability surfaces. These surfaces and the PES have then been used to calculate rovibrational intensities and demonstrate that the effects of an external electric field (a model for molecular environment) can be accurately approximated using a power series expansion and zero field property surfaces.

Reaction dynamics (Kable, Andrews, Quinn, Lee, Clubb, Hobday, Osborn (Sandia)): “Roaming” has been coined to describe a newly recognised class of reaction mechanism which bypasses the conventional transition state to a reaction. We have shown roaming mechanisms are ubiquitous, much more widespread than initially thought. We have also investigated triple fragmentation and photo-chemically-induced isomerization using both theory and experiment. We have shown that, under atmospheric conditions, acetaldehyde, \textit{CH}_3\textit{CHO}, can isomerise to vinyl alcohol, \textit{CH}_2=\textit{CHOH}, a precursor to formation of organic acids in the atmosphere. Notably we found at 1 atm pressure up to 26% of the acetaldehyde could undergo keto-enol isomerisation and this new mechanism may well explain the observed concentrations of organic acids in the atmosphere.

Computational drug design (Hunter (UNSW)): Fluorinated analogues of \textit{g}-aminobutyric acid (GABA) have been studied experimentally and modelled using quantum chemistry. These molecules act at GABA receptors in the central nervous system and are responsible for regulating neuronal firing. Theoretical modelling has characterised the different conformers of these analogues, their NMR spectra and their isomerization pathways. We found that the enantiomers of syn-2,3-difluoro-4-aminobutyric acid elicited opposite biological responses and we were able to interpret this in terms of our previously developed quantitative structure activity relationship (QSAR) for the GABAC receptor.

Above: (a) Potential Energy and Molecular Property Surfaces: \((b) (x, y, z) \textit{H}_3\textit{CNO}\), \((c) (x, z) \textit{H}_3\textit{CNO}\), and \((d) \textit{C}_0\textit{N}_0\textit{O}\) for \textit{ClH}:\textit{NH}_3

Above: A schematic showing energies (kJ/mol) and important structures on the \textit{CH}_3\textit{CDO} S\_0 PES. The green arrows indicate the experimental yields at 320 nm under collision-free conditions. At 1 atm we predict that excited acetaldehyde collisionally relaxes into both keto and enol forms as shown by the blue curvy arrows.
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.

Chemistry and biology of nicotinic receptors (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 of schizophrenia. We have developed structure-activity relationships strategies of the following small molecules in order to understand the motifs responsible for conferring \( \alpha_7 \) activity.

Chemistry of sigma receptors (Banister, Manohar, Manoli): 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 of 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.

Immunomodulation in the treatment and diagnosis of CNS disease (Narlawar, Hanani, Chau): The recognition that microglial activation is closely linked to the pathophysiology of brain disease has made the translator 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 P2X\(_7\) receptor in depression (Wilkinson, Law, Jackson, Barron, Werry): Over the last two decades there has been increasing evidence of a strong relationship between depression and immunological dysfunction in depressed patients. Excessive secretion of cytokines, such as interleukin-1\(\beta\) (IL-1\(\beta\)), and tumour necrosis factor-\(\alpha\) (TNF-\(\alpha\)) is increasingly recognised as a potential cause of depression. The purinergic P2X\(_7\) receptor modulates the maturation and release of cytokines such as IL-1\(\beta\) suggesting that the P2X\(_7\) receptor could play a role in the pathophysiology of depression and that blockade of the P2X\(_7\),R might result in antidepressant-like properties.

To date, only a few classes of drug-like molecules are known to interact with the P2X\(_7\),R. 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.

(Three-dimensional structure of TSPO by electron cryomicroscopy of helical crystals)
Temperature dependence of the oxygen occupancy in SrUO$_4$ compared to the TGA analysis

SOLID STATE AND MATERIALS CHEMISTRY

Defects and phase transitions

The perovskite NaTaO$_3$ shows promise as a photocatalyst for splitting water into H$_2$ and O$_2$. Cation doping is a powerful way to tune the band gap in perovskites and hence enhance the photocatalytic response, consequently efforts are being directed to understanding the correlation between the changes in the structure and photocatalytic properties upon doping. The flexibility of the perovskite structure allows for local defects whilst maintaining long range cooperative tilting of the corner sharing octahedra. High resolution synchrotron X-ray and neutron powder diffraction studies have demonstrated that, as prepared, NaTaO$_3$ is a mixture of two very similar orthorhombic phases and that the phase composition is extremely sensitive to the presence of dopants. In-situ diffraction studies are being used to establish the role of defects on the phase evolution and these studies will be used to guide optimisation of NaTaO$_3$ based photocatalysts. Partial replacement of the O in SrTaO$_3$ with N to form SrTaO$_3$N is another way of tuning the band-gap. We have identified that such doping disrupts the cooperative tilting of the TaX$_6$ octahedra leading to the formation of novel structures.

Magnetism in perovskites

We have established the crystal structures of the series of ordered double perovskites Ba$_{2-x}$Sr$_x$YRuO$_6$ (0 ≤ x ≤ 2) by high resolution synchrotron X-ray diffraction. Increasing the Sr content introduces tilting of the corner sharing octahedra $Fm\bar{3}m (d' a' d'' c')$, $\bar{4}3m (c' a' a' c)$ and $\bar{2}P2_1/n (a' a' a')$. The same sequence of structures can be induced by varying the temperature of appropriate members of the series. Magnetic susceptibility measurements demonstrate the oxides to be antiferromagnets with a Neel temperature of ~ 30K and we have identified a simple correlation between the Weiss constant $\theta$ and the Ru-O-Y bond angle.

Uranium oxides

SrUO$_4$ adopts two different structures depending on how it is made. We have found that under reducing conditions an oxygen deficient rhombohedral form $\alpha$-SrUO$_4$ is obtained and that the oxygen vacancies that are critical to the stability of the 8-coordinate UO$_8$ moieties, whereas under oxidizing conditions $\beta$-SrUO$_4$ is stoichiometric and has an orthorhombic structure with UO$_6$ groups. However the conversion of $\alpha$-SrUO$_4$ to $\beta$-SrUO$_4$ requires the sample lose still more oxygen! In-situ Synchrotron and Neutron Diffraction measurements have been used to study this bizarre behavior and we show that it is possible to stabilize the rhombohedral form to high temperatures.

Temperature dependence of the oxygen occupancy in SrUO$_4$ compared to the TGA analysis

PROFESSOR BRENDAN KENNEDY

Understanding how the structures of metal oxides change in response to stimuli is often the key in establishing structure-property relationships in functional materials. We use crystallography to study the impact of chemical substitutions on structural phase transitions and then correlate this with changes in the magnetic and electronic properties of the material.
MOLECULAR FRAMEWORK MATERIALS

Nanoporous molecular frameworks (Southon, Ragon, Keene, Duyker, Chen, Murphy, Barkhordarian, Ogilvie, Zenere, Zaiter, Peterson, McKenzie, 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 (Duyker, Wu, Chen, Cameron, Chadbourne, Ogilvie, 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 (Ragon, Clements, Zenere, Zaiter, Diwa, Mulaney, Sciorinto, Kirk, Klein, Price, Goux-Capes, Grünwald, Doheny, Hill, Southon, Halder, Murray, Mourbaraki, Létard, Brooker, Neville): 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 (Faust, Rizzuto, Walwyn, Doheny, Keene, Kanga, Murphy, 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.
MOLECULAR PHOTOPHYSICS

A model for exciton-polaritons in uniaxial molecular crystals (SCJ Meskers, G Lakhwani - University of Sydney, Eindhoven University of Technology): Strong light-matter interactions give rise to exciting emission properties, such as polariton lasing. Polariton laser is a type of electroluminescent device that can be powered by one-hundredth fraction of energy compared to a conventional laser. This property makes it extremely cheap and an effective coherent light energy source alternative for applications in biomedical imaging, high sensitivity security sensors and optical communications. Inside a material, a photon hybridizes with electronic excitations to form an exciton-polariton. The exciton-polariton has three available spin states or polarizations, while a photon in vacuum has only two. This change in the number of internal degrees of freedom is related to breaking of the gauge symmetry for the photon when going into polarizable matter where the speed of propagation of the energy quantum is reduced to below c. We argue that when calculating reflection and refraction of light at the vacuum/matter interface, a uniform gauge condition should be applied across the interface. This condition allows for a solution of the infamous additional boundary condition (ABC) problem in the optics of condensed matter. We show that experimental reflection spectra from molecular crystals can be reproduced accurately. In addition, we predict a later displacement of a light beam reflected externally at the vacuum/matter interface with respect to the incoming beam, an effect known as the Goos-Hänchen shift. Furthermore, the model predicts the occurrence of trirefringence, i.e. the refraction of an incident light beam into three separate beams with different polarizations when entering an anisotropic material (see Fig 1).\textsuperscript{1,2}

2. SCJ Meskers, G Lakhwani submitted (2016).

Fig 1. Trirefringence at the vacuum-matter interface giving rise to three separate polarized beams. The polarization of the matter is described both on a macroscopic scale (bulk current density $J$) and at the microscopic level (local current density, $j$). The microscopic current sources are dipole oscillators positioned on a cubic lattice with lattice constant $\Delta$ and oriented in the $i$ or $x$ direction.

Fig 2. Chemical structures of the F8T2 derivatives P1, P2 and P3 with fluorene unit marked in black and bi-thiophene in red. The schematic drawing (inset) shows interchain stacking.

DR GIRISH LAKHWANI

Our research focuses on developing spectroscopic methods to understand bottom-top nanoscale build-up of morphology and photophysical properties originating at different length scales in $\pi$-conjugated materials for applications in optoelectronic devices.

Aggregation control and its effect on the photophysics and charge transport (B Freidel, G Lakhwani – University of Sydney, Graz University of Technology): In organic photovoltaics, thin-film morphology is critical in determining the photophysical properties of devices. For example, ordering of conjugated polymers is required to facilitate efficient energy and charge transport, however, strong aggregating behavior leads to formation of grain boundaries that act as charge traps. In this work, we have synthesized two types of poly(9,9-dioctylfluorenyl-co-bithiophene) (F8T2) with different side-chains on the backbone of equal number of carbons - while the straight octyl chains have the ability to interdigitate in a “zipper-like” structure and thus crystallize very strongly, branched side-chains are more bulky, thus force a larger backbone distance in the interplanar and the head-to-head (“end-to-end” stacking) direction (see Fig 2). Photovoltaic characteristics of these donor polymers were studied in conjunction with ICBA as acceptors with latter polymer displaying higher (~ two orders) charge carrier mobility.\textsuperscript{3}

Our research is focused on biomedicine including: the design and understanding the mode of action of anti-cancer and anti-diabetes drugs; biospectroscopic studies on disease processes, disease diagnostics, and the efficacy of new treatments.

**BIOINORGANIC CHEMISTRY**

Anti-diabetic effects of chromium, vanadium, molybdenum, and tungsten (Carter, Glover,* Harms,* Kaur, Khani, Lee, Levinia, Saffrom, Wood): Research has continued on empirical methods for determining the structures and speciation of Cr, Mo and V complexes in biological fluids, cells, and tissues. This has included the biotransformations of anti-diabetic drugs and supplements. Research has continued on Cr(V) sugar complexes using X-ray crystallography and theoretical calculations to correlate specific isomers with their properties.

Vibrational spectroscopic microbe techniques and immunoblotting assays have been used to provide further evidence that Cr(VI), Cr(V), Mo(VI), V(V), W(VI) inhibit phosphatase enzymes within target adipocytes (fat cells), muscle cells and liver cells, which is probably a major cause of the anti-diabetic activities of Cr, Mo, V and W anti-diabetic supplements and drugs. Extensive studies on intracellular sugar metabolism and the effects of these metals on the metabolism have been conducted with Seahorse technology on bulk cells and vibrational spectroscopy on single cells. The BLItz technique has also been used to test how metal binding changes the transferrin (Tf)/ transferrin receptor (Tfr) and insulin/insulin receptor interactions. Surprisingly, binding of metals to Tf inhibits rather than increases metal uptake, which shows that other transport mechanisms are important.

Ga, Rh and Ru and V anti-cancer drugs (Andrews,* Baker, Bebawy,* Biro,* Carter, Chen,* Chetcuti, de Jonge,* Dinda,* Finney,* Levinia, Liang, Luk,* Markham, O’Riley, Paterson,* Tobin,* Turner, Vogt,* Wood): Research was 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 (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. Extensive studies have been undertaken with cancer microparticles (microvesicles) released by cancer cells, which are important in drug resistance and cancer progression and metastases. These have revealed a heterogeneous population, which may have different roles in the disease. We are also investigating their potential to target cancer cells.

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

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 and the BLItz technique to examine modifications of Tr/Tfr interactions, which are also modified substantially by fluorophore labelling of Tr.

**Disease diagnosis and differentiation in cells and tissues** (Aitken, Banati,* Carter, Chen,* de Jonge,* El-Assaad,* Graeber,* Grau*, Hackett, Hunt,* Lee, Levinia, McQuillan,* Pamphlett,* Paterson,* Vogt*): Vibrational spectroscopic diagnostics for various diseases and conditions: including cerebral malaria; bacterial and viral meningitis, sleep apnea treatment; and Parkinson's 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. Vibrational spectroscopic mapping and imaging were used, together with synchrotron X-ray microprobe techniques, to understand the disease biochemistry of some of diseases of the brain and the role of microparticles derived from monocytes on septic shock.

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**PROFESSOR PETER LAY, FAA**
MATERIALS CHEMISTRY; NEUTRON & X-RAY SCATTERING SCIENCE

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 to discover, characterise and optimise functional solid-state materials. Structure 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 conduction in large single crystals

The high-temperature cubic form of bismuth oxide, δ-Bi₂O₃, is the best intermediate-temperature oxide-ionic conductor known. The most elegant way of stabilizing δ-Bi₂O₃ to room temperature, while preserving a large part of its conductivity, is by doping with higher-valent transition metals to create wide solid-solutions fields with exceedingly rare and complex (3+3)-dimensional incommensurately modulated “hypercubic” structures. These materials remain poorly understood because no such structure has ever been quantitatively solved and refined, due to both the complexity of the problem and a lack of adequate experimental data. We have addressed this by growing a large (cm-scale) crystal using a novel refluxing floating-zone method, collecting high-quality single-crystal neutron diffraction data, and treating its structure within the superspace symmetry formalism. The structure can now be understood as an “inflated” pyrochlore, in which corner-connected NbO₆ octahedral chains move smoothly apart to accommodate the solid solution. While some oxide vacancies are ordered into these chains, the rest are distributed throughout a continuous three-dimensional network of wide δ-Bi₂O₃-like channels, explaining the high oxide-ionic conductivity compared to commensurately modulated phases in the same pseudo-binary system.

Giant magnetoelectric effect in 5d oxides

Negative thermal expansion (NTE), where the volume of a material expands anomalously on cooling, can arise through a range of mechanisms. Some are essentially mechanical, based on the thermal motion of coupled rigid units (e.g., ZrW₂O₈), while others involve a redistribution of electron density, often associated with changes in magnetic properties (e.g., the Ni-Fe alloy known as Invar). The compound Ba₃BiIr₂O₉ is an entirely novel case of the latter, magnetoelectric, case. Its structure contains face-sharing Ir₂O₉ bi-octahedra with direct bonds between Ir⁴⁺ cations. On cooling through $T^* = 74$ K, the length of this Ir–Ir bond suddenly increases by 4%, producing a giant 1.0% volume NTE, accompanied by a sharp drop in magnetic susceptibility. The transition appears to be driven by a dramatic change in the interactions among Ir 5d orbitals, at the crossover between two competing ground states: one that optimises direct Ir–Ir bonding (at high temperature); and one that optimises Ir–O–Ir magnetic superexchange (at low temperature).

ASSOCIATE PROFESSOR
CHRIS LING

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.
PROFESSOR THOMAS MASCHMEYER, FAA FTSE

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.

ADVANCED CATALYSIS FOR SUSTAINABILITY

Sustainable chemistry and processes: 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 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 as 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, TiO₂-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.
ORGANOMETALLIC CHEMISTRY AND CATALYSIS
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 processes, 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.

Highly efficient catalysts for deep hydrogenation: Deep hydrogenation of aromatic substrates under mild conditions is a technically demanding, but most important problem impacting on two sustainability issues – the quests for greener fuels and for hydrogen storage materials. Emerging environmental legislation requiring the removal of aromatics from gasoline can be met by arene hydrogenation. Liquid organic hydrogen storage materials compatible with existing infrastructure are attractive and require hydrogenation/dehydrogenation catalysts which can operate under mild conditions. We have developed a sulfur-resistant multimetallic catalyst able to hydrogenate toluene under near ambient conditions in water.

Catalysts for the hydrogen evolution reaction: The hydrogen evolution reaction (HER, H+ + e- ↔ ½H2) is one of the main routes for the production of molecular hydrogen. This electrochemical process can be made environmentally sustainable by combining the reaction with a source of renewable electricity. Presently, the most efficient catalysts for the HER are noble metals such as platinum. However the reserves of these metals are insufficient to meet projected needs, so it is important to find alternative electrocatalytic materials that are highly active, yet inexpensive and abundant. We have developed several solid and molecular HER electrocatalysts.

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 Redflow, 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 nanocapsulation, and sulfur tolerant reforming catalysts.
On-water chemistry (Phippen, Norcott, Beare, Graham): Water is the most abundant liquid on our planet – we are surrounded by it. Yet when it comes to reactions, chemists traditionally use toxic, flammable and expensive fossil-fuel based solvents. We are working to change that. Environmental and safety considerations have led us to consider water as the ultimate solvent in which to perform chemical reactions. Despite the fact that most organic compounds are insoluble in water, some organic reactions are actually faster when performed “on water”. We have recently uncovered the explanation for this unusual phenomenon and have employed “on water” catalysis to facilitate the total synthesis of complex natural products and drug-like molecules [Tetrahedron Lett. (2013) 54, 1056–1058]. We have even used water to catalyse trans-formations such as the aromatic aza-Claisen rearrangement [Org. Biomol. Chem. (2013) 11, 2452–2459]. And finally, we have married the sustainable nature of water-based methods with the burgeoning potential of ionic-liquids to allow two insoluble materials to react under mild conditions [Chem. Commun. (2013), 49, 8347–8349].

Extending the scope of the Stetter reaction (Law, Bromhead, Daridis): Building molecules means forging new carbon-carbon bonds. The Stetter reaction is an organocatalytic umpolung process in which aldehydes (which are normally electrophilic) become nucleophilic and add to alkenes. The Stetter reaction can form multiple stereogenic centres in an enantioselective fashion, but it is seldom used in synthesis. We are trying to change that mindset. We are employing the Stetter reaction as the key bond-forming process for the synthesis of important plant signalling molecules. Working closely with researchers in Japan and Israel, we are designing and building molecules that affect how plants grow, how seeds germinate and how plants interact with fungi in their local environment. We are also increasing the usefulness of the Stetter reaction by inventing new modes of reactivity. We recently reported the vinylogous Stetter reaction, a process which builds up molecular complexity in a single, enantio-selective operation [Chem. - Eur. J. (2013) 19, 15852–15855]. This new process will make the synthesis of some imposing molecular architectures much more straight-forward.

Synthesis of bromine-containing natural products (Recsei): There are some reactions that occur in nature that we simply cannot perform in the laboratory. The brominative cyclization of terpenes is an important example. Even though this reaction produces compounds with vast agrochemical potential, we can’t do it in a flask... until now. Over the past few years the group has spent time developing a new class of binol-derived catalysts that allow the diastereoselective cyclization of simple starting materials to give a range of important compounds. For the first time, this new process gives ready access to the snyderane class of bromine-containing natural products. We have recently used this new process to complete the inaugural synthesis of (+)-luzofuran.
The main research focus of the group is the design of macromolecular architectures that assist the synthesis of novel hybrid materials, self-assembled sensors or tailor-made nanoparticles for drug delivery and biomedical applications.

**FUNCTIONAL POLYMER NANOPARTICLES**

**Molecular bottlebrushes *in vivo*:** Studies of spherical nanoengineered drug delivery systems have suggested that particle size and mechanical properties are key determinants of in vivo behaviour; however, for more complex structures, detailed analysis of correlations between *in vitro* characterization and *in vivo* disposition is lacking. Anisotropic materials in particular bear unknowns in terms of size tolerances for *in vivo* clearance and the impact of shape and rigidity. We employed cylindrical polymer brushes (CPBs) to answer questions related to the impact of size, length and rigidity on the behaviour of PEGylated anisotropic structures, in particular their pharmacokinetics and biodistribution. A modular grafting assembly allowed for the systematic tailoring of parameters such as aspect ratio or rigidity while keeping the overall chemical composition the same. Water-soluble, low-fouling CPBs with altered length were produced and radiolabelled, which subsequently allowed us to follow the pharmacokinetics of intravenously injected CPBs as well as their deposition into major organs. To alter the rigidity of the CPBs, core-shell-structured CPBs with a crystalline polycaprolactone core were synthesized (Figure 1). This modular build-up of CPBs allowed their shape and rigidity to be altered, which in turn could be used to influence the *in vivo* circulation behaviour of these anisotropic polymer particles. Increasing the aspect ratio or altering the rigidity of the CPBs led to reduced exposure, higher clearance rates, and increased mononuclear phagocytic system (MPS) organ deposition (*ACS Nano* 2015, 9, 1294-1304).

**Brush nanoparticles for drug delivery:** Polymer brush nanoparticles offer great control over composition and functionality. In this project we have furnished charge-neutral hydrophilic molecular polymer brush nanoparticles with the ability to host cytotoxic drugs and release them upon acidification. Once internalised into cancer cells, the nanoparticles experience a drop in pH within intracellular compartments which triggers the drug release. The microscope image (Figure 2) indicates the release of drug molecules (red) within the cells. Cell nuclei are stained blue and appear pink once the drug molecules have entered the cell nuclei.

**Modular design of charge-neutral polymer particles:** In this work, we reported a templating approach for the preparation of functional polymer replica particles via surface-initiated polymerisation in mesoporous silica templates. Subsequent removal of the template resulted in discrete polymer particles. Furthermore, redox-responsive replica particles could be engineered to disassemble in a reducing environment. Particles, made of zwitterionic or PEG-based polymers, exhibited very low association to human cancer cells, which rendered these charge-neutral polymer particles a modular and versatile class of highly functional carriers with potential applications in drug delivery (*Langmuir* 2014, 30, 6286). Moreover, this modular method can be used to produce core-shell polymer nanoparticles with a drug loaded core (red) and a hydrophilic biopolymer shell (green) (Figure 3).
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.

**Nano Interfaces**

New polymer patterns through solvent annealing (Al-Khayat, Beck, Shou, Geraghty, Hong, Thickett): In our effort to optimise micropatterned polymer surfaces that collect water from the atmosphere, we have engineered topographies of different surface chemistry and size. We are now able to tune the size of the dewetted patterns from a few hundred nanometers to hundreds of micrometers, using very thick films that previously were considered stable (micrometer thick). This tunability allowed us to quantify the dimensions and density of features that lead to the higher water collection ability, in different environmental conditions. We have developed more accurate ways to quantify water collection efficiency using a purpose-built condensation chamber (Fig. 1).

Robust self-assembled monolayers on different solid substrates (Shou, Wood, Chisholm, Cashman): We have demonstrated that stable and compact monolayer films can be formed on solid surfaces using a previously untapped intermolecular interaction. The strong adsorption of perfluorinated alkanes produces hydrophobic surfaces with extremely low free energy, which are stable from room temperature to temperatures as high at 150°C, but desorb when wetted by protic solvents. This new family of self-assembled monolayer could find ideal application in the electronic field, where use of protic solvents is deleterious for high efficiency.

Superhydrophobic surfaces through film wrinkling (Scarratt, Hawkett, Jiao): Superhydrophobic surfaces formed through the spontaneous wrinkling of a rigid Teflon film deposited on a shrinkable substrate were fabricated and their mechanical properties investigated. The produced wrinkled surfaces are highly robust to scratching and indentation, due to the interpenetration between the teflon film and the underlying structure. Their robustness compares well with commercial coatings used currently for different advanced applications (Fig. 2).

Polymeric Janus nanoparticles (Hawkett, Duong, Nguyen): The synthesis of all-polymeric Janus nanoparticles has been refined to the point where we can now tune the size and chemistry of each lobe, with the capacity to stabilize emulsion droplets of different oils, and to form films under controlled conditions. This control has opened a completely new paradigm in the use of Janus particles as solid emulsion stabilizers that are much more stable and offer multiple functions, as we are exploring in an ARC Linkage grant co-funded by Dulux Australia.

**Associate Professor Chiara Neto**

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.
Our research is aimed at embedding magnetic switching centres into metal-organic polymeric materials towards generating binary switches and molecular sensors. Through understanding the structure and functional properties of these new materials we strive to fine-tune switching behaviours and uncover novel magnetic characters.

**SPIN CROSSOVER SYSTEMS**

**Predictable multi-stability** (Sciortino, Ragon, Zenere, Zaiter, Richards, Murphy, Létard, Chastanet, Murray, Kepert): The spin crossover phenomenon is a prime example of bistability as two electronic states are possible at the same temperature. Some spin crossover materials can show multiple steps and are of considerable interest as they provide access to additional stable electronic states for expanded information storage capacity. In this project we endeavor to create a consistent platform for producing spin crossover materials which display multiple steps through generating multiple spin switching sites in the one material. Through this approach we have successfully developed a large family of porous spin switching materials that consistently show multiple stepped spin transitions. Detailed structural studies show a strong correlation between an asymmetric ligand binding mode, strong host-guest interactions and the overall production of multiple spin switching sites. This has allowed us to tailor solid state interactions to generate record breaking two-stepped transitions such as a 130 K thermal stability region of mixed spin states (Figure 1). Further asymmetric functionalization of the organic ligands is proving to be a feasible method for producing rare three- and four-stepped transitions.

**Flexible porosity** (Sciortino, Kepert): To date with continued thermal cycling (i.e., repeated heating and cooling) the majority of spin crossover materials show consistent magnetic properties. In this project we are harnessing the unique features of flexible framework scaffolds and the significant volumetric change of spin crossover to generate materials with dynamic magnetic properties. We are utilising both the interplay between flexible host lattices and between host framework and guest molecules to explore this novel phenomena. With significant success in this respect, we have seen emergent sensing applications such as a thermal reset feature (i.e., temperature sensor) and a thermal cycling counting function.

**Photo-active ligands** (Ragon, Sciortino, D’Alessandro, Létard, Chastanet, Kepert): Spin crossover materials are most commonly perturbed using thermal variation. This project involves the incorporation of photo-active ligands into spin crossover materials in order to switch magnetic states using only the application of light-irradiation. Most importantly this may allow spin switching to occur at ambient temperatures. Using porous metal-organic frameworks as a platform and including photo-active ligands with pendant functional groups which protrude into the pore space a pseudo-solution state environment can be generated for enhanced photo-activity.
The main research focus of the group is the development of chemical tools to assist the study of biological systems. Chemical synthesis holds the key to uncovering molecular interactions within cells, which cannot be probed by conventional imaging techniques. We are mainly interested in preparing fluorescent sensors for use in confocal microscopy and flow cytometry, and in developing responsive contrast agents for magnetic resonance imaging (MRI).

### CHEMICAL PROBES FOR BIOLOGY

**New fluorescent sensors for the study of oxidative stress in biology (Carr, Fraser, Jankowska, Kaur, Kolanowski, Yang):** Many diseases are associated with perturbations in redox state, so developing ways to measure biological oxidation state will help us to better understand these diseases and suggest ways to cure or treat them. We have extended our toolbox of reversible fluorescent sensors for cellular redox state, developing mitochondrially-targeted sensors, and ratiometric reporters (Chem Commun., 2015, 51, 10510; Org. Biomol. Chem., 2015, 13, 6686; Antioxid. Redox Sign., 2016, DOI: 10.1089/ars.2015.6495). Our probes have demonstrated utility in various cellular and multicellular models, including tumour spheroids and *C. elegans*. We have also developed simple methods to target such probes to other sub-cellular organelles, including the peroxisomes and Golgi apparatus.

**Magnetic resonance sensors of redox state (Bonnitcha, Jankowska, Kolanowski, O’Neill):** Magnetic resonance imaging (MRI) offers the possibility of high resolution, whole animal imaging. We have developed a gadolinium-based MRI contrast agent that signals oxidative stress, and the first cobalt-based MRI contrast agent capable of reporting on hypoxia (RSC Adv., 2016, 6, 30021).

**Tools to study labile pools of metal ions (Carney, Kolanowski, Shen, Smith):** The pool of labile, or bioavailable, metal ions in a cell is crucial to the function of metalloproteins and the maintenance of metal homeostasis. We are developing probes for biologically-relevant metal ions, that can be used to provide information about how labile metal pools change in conditions of health and disease. For example, we have developed a ratiometric fluorescent sensor that reports on mitochondrial copper levels.

**Fluorescent sensing arrays for metal ions (Carney, Smith):** Detection of heavy metals in waterways or in body fluids requires achievement of high selectivity, even in the presence of other potentially-interfering ions. Fluorescent arrays enable study of complex solutions of analytes through the use of a set of fluorophores, which give a fingerprint response to a specific analyte. We have developed novel arrays using small molecule fluorophores that are capable of distinguishing heavy metals in solution (Analyst, 2016, in press).

**New methods to fluorescently-sense platinum (Dawson, Hambley, Lim):** Platinum-based anticancer agents play an important role in chemotherapy, but their interactions with cells remain poorly understood, highlighting the need for new tools to study Pt in cells. We have prepared new sensors of platinum metabolites, including trans-platinum species.

**Understanding the relationship between platinum-based chemotherapy and copper homeostasis (Akerfeldt, Hambley, Lim, Tran):** Cisplatin and its analogues are reported to interact with the copper transport protein, Ctrl, but little is known about their effect on copper homeostasis more broadly. We are investigating this relationship in order to better understand how cisplatin acts as a chemotherapeutic agent, and how its efficacy can be improved.
**Tuberculosis drug discovery** (Dowman, Elias, Giltrap, Hawkins, Tran, Watson, Britton): Mycobacterium tuberculosis, the etiological agent of 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 recently discovered a number of new TB drug leads via the use of structure-based inhibitor design and through the synthesis of natural products and natural product analogues (e.g. Org. Lett. in press).

**Total synthesis of marine natural products as novel antimalarials** (Chung, Stoye, Hunt, Rosenthal): 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 gallinamide A, isolated from a marine cyanobacterium (Chem. Eur. J. 2011, 13544). A library of gallinamide A analogues have now been synthesized and several have exhibited more potent antimalarial activity than the frontline antimalarial therapy chloroquine (J. Med. Chem. 2014, 10557).

**Synthetic glycopeptides as cancer vaccine candidates** (Artner, Corcilius, McDonald, Stanojevic, Byrne): 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 developed novel chemistry for the synthesis of TACA-derived amino acids (Org. Lett. 2013, 5794) and for the generation of a library of self-adjuvanting, multi-component glycopeptide cancer vaccine candidates. We have shown that these vaccines provide strong and sustained antibody responses against tumour-associated epitopes in mice models (Chem. Commun. 2014, 10273, Front. Chem. Biol. 2015).

**New methods for the chemical synthesis of therapeutic proteins** (Liu, Mitchell, Premjdee, Sayers, Wang and Wang): Peptides and proteins mediate a number of important biological functions and therefore represent attractive candidates for novel therapeutics. The development of concise synthetic routes to these complex targets is essential for pharmaceutical application. We have developed a number of new synthetic ligation strategies that enable the rapid and efficient construction of peptide and protein targets (Chem. Sci. 2014, 260, Curr. Opin. Chem. Biol. 2014, 70, Org. Lett. 2015, 2070, Angew. Chem. Int. Ed. 2015, 12716, J. Am. Chem. Soc. 2015, 14011, Acc. Chem. Res. 2015, 2251). We have further demonstrated the utility of these techniques through the total synthesis of homogeneous variants of antithrombotic proteins including hirudin P6 from medicinal leeches (Angew. Chem. Int. Ed. 2014, 3947) and madanin-1 and chimadanin from bush ticks (J. Am. Chem. Soc. 2014, 8161). We are currently evaluating the therapeutic potential of synthetic protein analogues based on these motifs.

**Group news:** 2015 saw the arrival of a number of new group members including Luke Dowman, Wendy Tran and Vicki Stanojevic (Honours), Jess Sayers (PhD) and Eileen Wang (PhD). We also welcomed back Emma Watson and Jonathan Chung as PhD students after completing their honours year in the group in 2014.
BIOINORGANIC MEDICINAL CHEMISTRY
Our research group has a strong interest in the development of new boron and lanthanoid agents for application in medicine, particularly in cutting-edge cancer treatments known as Neutron Capture Therapy (NCT) and Photon Activation Therapy (PAT). To date, we have discovered several new classes of DNA-, mitochondrial- and tumour-targeted compounds and we are actively exploring their potential as PAT and NCT agents. We are also actively exploring the application of boron clusters, in particular the carboranes, as unique types of structural frameworks in medicinal chemistry.

New gadolinium agents for binary cancer therapies (Busse, Fenton, Hall, Harris, Kardashinsky, Morrison): A recent breakthrough made by our group opens up new horizons in the delivery of Gd to tumour-cell mitochondria for potential application in binary therapies involving PAT or NCT. We recently reported a new class of Gd(III) complexes with the necessary characteristics for efficient tumour targeting by exploiting a mitochondrial uptake mechanism. Such agents display low in vitro cytotoxicity in the absence of neutrons/photons and a high propensity to accumulate within the mitochondria of human brain tumour (T98G) cells. Our prototype Gd(III) complex also exhibits a high degree of selectivity (24 : 1) for T98G cells over normal, human glial (SVG p12) cells. Significant numbers (> 10⁸) of Gd atoms (equating to ca. 3 x 10⁵ ppm) can also be delivered to a single T98G cell. Importantly, recent in vitro PAT experiments involving the prototype Gd(III) complex and synchrotron X-ray photons (60 keV) demonstrate an unprecedented level of T98G cell kill and selectivity in the presence of both the Gd(III) complex and synchrotron X-ray radiation.

Carboranes as unique structural frameworks in medicinal chemistry (Austin, Kahlert, Kassiou, Narlawar, Wilkinson): A lack of structural diversity in potential drug candidates has been cited as a serious bottleneck in the drug discovery process. This factor alone has severely limited exploration of the so-called biologically-relevant “chemical space” over the past century. The unique chemistry of boron offers great promise in expanding the size and scope of biologically-relevant “chemical space” in the search for novel drug leads. We are currently evaluating the application of robust boron clusters (in particular, the carboranes) as unique structural elements in drug design. To date, we have developed the first boron agents that can target the indoleamine-2,3-dioxygenase-1 (IDO1) enzyme which is directly involved in tumour immunity escape, the translocator protein (TSPO) which plays important roles in steroidogenesis and the regulation of cell growth, differentiation, and apoptosis, and we have also recently reported the first example of a boron-based drug exhibiting CNS-modifying effects in vivo by targeting a brain receptor known as the P2X₇, with direct implications in CNS diseases such as depression.

New boron fluorophores for near-IR biological applications (New, Wu): Fluorescently-labelled molecules are invaluable tools in microscopy. There is a continuing need to develop new types of fluorophores, particularly those that emit in the near-IR. This project involves the rational design and synthesis of new boron-containing fluorophores, their photophysical characterisation and also biological studies. Recently, we developed the first coumarin derivatives containing a carborane cage. All these compounds showed excellent hydrolytic stability and intriguing luminescence properties in aqueous solution.

Our research group is primarily interested in the medicinal chemistry of boron and the lanthanoid elements, particularly gadolinium.
METAL-BASED THERAPEUTICS

Almost half of all drug candidates that enter clinical trials fail due to problems such as poor bioavailability, low efficacy and severe side effects. Synthetic modifications to overcome these limitations are often difficult and require a large number of synthetic steps. An alternative approach is to deliver the drug as a metal prodrug complex. This is a synthetically simple strategy that can improve both the pharmacokinetic and pharmacodynamic properties of the parent drug. With a wide range of potential ligands and diverse synthetic chemistry, metal complexes represent versatile scaffolds that can be tailored to overcome the specific limitations of a broad spectrum of drugs.

Targeting oxygen deficient tumour regions with redox active metal complexes (Oxman): One of the distinctive characteristics of many transition metal complexes is a large difference in lability between different oxidation states. Our interest is in exploiting this feature to develop inert complexes that are reduced to a labile form in the oxygen deficient, reductive environment found in many solid tumours.

We have investigated cobalt(III) and ruthenium(III) complexes for this purpose. Using a combination of fluorescence lifetime imaging and X-ray absorbance spectroscopy, we demonstrated that a cobalt(III) prodrug complex of the anticancer drug curcumin preferentially releases curcumin in oxygen deficient tumour cells through reduction to a labile cobalt(II) complex (Renfrew et al. Chem. Sci. 2013).

We have also investigated the use of visible light as a means of releasing a drug from a cobalt(III) prodrug, showing that inert cobalt(III)-curcumin complexes can undergo ligand exchange to release curcumin when irradiated with visible light. This is the first example of a cobalt complex for the caging and light-activated release of a biomolecule. (Renfrew et al. Chem. Eur. J. 2015).

Ruthenium complexes for photoactivated chemotherapy (Chan, Karaoun, Wei): Photoactivated chemotherapy, the use of light to activate a non-toxic prodrug, is an evolving technique for the localised treatment of diseased tissue. These ruthenium complexes form very stable complexes with a range of N-heterocycle containing drugs. Only when the ruthenium-prodrug is irradiated with green light is the metal-drug bond cleaved and the active drug released. We have demonstrated the versatility of this strategy by developing ruthenium prodrugs of a range of different drugs including pyridine-based growth factor inhibitors, 1,2,4-triazole-containing oestrogen synthesis inhibitors, and imidazole antifungal agents. We have recently developing the first ruthenium complex able to selectively release an imidazole-based drug with green light irradiation (N. Karaoun et al. Chem Commun. 2015). (Figure 1).

Metallo drugs to target resistant bacteria (Lo): With increasing incidences of bacteria that are resistant to many or all known antibiotics, there is an urgent need to develop new treatments to combat bacterial infections. In collaboration with Dr Alysha Elliot at the University of Queensland, we have developed a class of ruthenium-based therapeutics with very selective activity towards resistant gram positive bacteria. The complexes are non-toxic towards human cells but inhibit methicillin-resistant Staphylococcus aureus growth at nanomolar concentrations. In related work, we are working with A/Prof Jamie Triccas at the Charles Perkins Centre on developing metal-based drugs to target resistant tuberculosis.

Our research focuses on using stimuli-responsive transition metal complexes for controlled and selective drug delivery.
There is another aspect of sugar molecules, which makes them really interesting. Most often, when we talk about sugar, we are referring to a mixture of glucose and fructose, both simple sugars. Apart from providing energy as the body’s main source of fuel, some of these simple sugars get modified in our body into complex sugar structures—macromolecules. Some glucose is converted to ribose or deoxyribose, essential building blocks of important macromolecules, such as RNA, DNA and ATP. Cells from higher animals and various microorganisms produce sialic acid in a long pathway starting from glucose. This nine-carbon sugar rarely occurs in free state in nature and it is more commonly present as components of oligosaccharide chains of mucins, glycoproteins, and glycolipids. It usually occupies terminal, nonreducing positions of oligosaccharide chains of complex carbohydrates on outer and inner membrane surfaces in various linkages, where it is highly exposed and functionally important. Some glucose is metabolized into sugar donor unit (UDP-GlcNAc), which is utilized by carbohydrate processing enzymes to decorate proteins with sugars to expand protein functions through process called post-translational modification (PMT). The list biological transformation and use of glucose is endless.

The flu viral enzyme sialidase (the “N” of H5N1) acts as a pair of biological scissors clipping sialic acid residues from the surface glycoproteins of the newly synthesised virion progeny and the infected host cell surface. This action facilitates viral infection. Using 3D structure of enzyme, sialic acid analogues are developed that can selectively target and inhibit conformation of viral protein sialidase present in highly pathogenic “bird flu” and recent pandemic “swine flu” viruses. These sugar analogues are important tools to develop next generation influenza therapeutics and also have potential to predict future flu pandemics.

My research interests lie in the area of chemical biology. The current research focus of the group is development of reagents for studying carbohydrate processing enzymes and carbohydrate binding proteins to probe problems of medicinal and biological significance. Essential mammalian enzyme O-GlcNAc transferase (OGT), regulates numerous cellular processes through the attachment of sugar residue to acceptor molecules - intracellular proteins through process called PMT. Several hundred proteins (~4000) involved in a wide range of cellular functions are modified with O-GlcNAc by single enzyme OGT. Unlike other PMT such as phosphorylation, where we have more than 500 protein kinases to modify similar set of proteins with a phosphate group. Aberrant OGT activity is a feature of several cancers. Taking inspiration form the nature, the group is using novel approach to produce first generation of inhibitors of the enzyme – bisubstrate analogues. Tunicamycin antibiotic is natural bisubstrate inhibitor in which donor and acceptor analogues are covalently attached to each other. The rational design of bisubstrate analogue inhibitors is being carried out using information about the enzyme’s 3D structure. The idea is to develop these inhibitors as cell-permeable inhibitor probes which will allow studying role of this enzyme in cancer. These probes will also have numerous applications in cancer diagnosis. These snapshots demonstrate that sugars are fascinating molecules of life sciences.

Carbohydrates, unlike DNA, RNA and proteins, can form branching structures and exhibit a mind-boggling diversity of structures and functions. We often hear someone saying, ‘I want to reduce my sugar intake!’ or we always look for sugar contents on food products at the supermarket. Why are we so worried about sugar, is sugar really that bad? It’s not all bad!
BIO-INSPIRED SYNTHESIS AND CHEMICAL BIOLOGY

Antibiotics chemistry: In September we welcomed Dr Malcolm Spain as a post-doctoral fellow to spearhead work on our NHMRC-funded project A new class of inhibitors for the treatment of tuberculosis (APP1084266, Triccas, Rutledge, Todd and West, 2015–2017). Work continues apace to map out structure/activity relationships in these unusual antitubercular agents, and to elucidate a mechanism of action (with Malcolm Spain, Mingfeng Yu, Hasini Murage, Daniel Moawad, Gaya Nagalingam, Mat Todd, Jamie Triccas and Nick West).

In the area of antibiotics biosynthesis and discovery, the search continues for new antibiotics from marine organisms (with Mozhdeh Dinarvand, Diana Quan, Ceri Jennings and Jamie Triccas) and we published two important reviews in 2015: a chapter on penicillin biosynthesis in the Royal Society of Chemistry’s new book 2-Oxoglutarate-Dependent Oxygenases (RSC Publishing, Cambridge, pp. 414-424); and a review of natural products discovery by activation of silent biosynthetic gene clusters (with Greg Challis, Nature Rev. Microbiol. 13 509 (2015), see figure), arising out of my sabbatical visit to Warwick in 2012.

Chemical sensing: We continue to work on fluorescent systems for monitoring pH and metal ions in vivo, and for visualising interactions between small molecule ligands and biomolecular targets. Exploring the fluorescence behaviour of naphthalimide- and coumarin-appended cyclam conjugates we have elucidated the basis for differences in their observed responses to zinc(II) and copper(II) (Eur. J. Inorg. Chem. 2015 58 (2015), with Sandra Ast, Stefanie Kuke and Mat Todd).

Our attempts to incorporate BODIPY fluorophores in these systems led to the discovery of a new method for the selective removal of boron from F-BODIPY derivatives (Beilstein J. Org. Chem. 11 37 (2015), with Mingfeng Yu, Joseph Wong, Cyril Tang, Peter Turner and Mat Todd).


Biomimetic chemistry: The selective functionalisation of hydrocarbons using biocatalytic and biologically inspired methods is another area of ongoing interest. In 2015 we published the first report of non-heme iron mimetics that catalyse allylic amination reactions, i.e. C–N bond formation (Beilstein J. Org. Chem. 11 2549 (2015), with David Porter and Belinda Poon), and the synthesis of new amide ligands for these and related reactions (Scientific Reports 9 9950 (2015), with Prarthana Devi, Sarah Barry, Kate Houlihan, Michael Murphy, Peter Turner and Paul Jensen).
INORGANIC SOLID STATE CHEMISTRY AND CHEMISTRY EDUCATION RESEARCH

View from the inside of a rechargeable Li-ion battery (Brant): In order to understand the processes that directly affect the properties of a rechargeable battery, in-situ analyses are essential. In-situ data collected at the Australian Synchrotron allow us to correlate structural changes with the electrochemical behaviour. In addition, the fast data collection times possible at a synchrotron source enable us to obtain real-time kinetic data. Our in-situ cell was used to investigate the insertion and removal of lithium for the defect perovskite $\text{Li}_{0.18}\text{Sr}_{0.66}\text{Ti}_{0.5}\text{Nb}_{0.5}\text{O}_3$. Figure 1 shows the “breathing” of the material as it first expands to insert lithium into the crystal structure, and then contracts again as lithium is removed. Further, due to the rapid data collection, additional subtle changes in the expansion were observed. That is, the rate of expansion is not constant, although the rate of lithium insertion is constant. These changes can be correlated with changes in the slope of the voltage profile.

Towards sustainable energy storage (Murphy, Godfrey, Kepert, Kuhn†): Interest has been growing in the development of Na-ion batteries, due to abundance of Na (compared to Li) and safety aspects. Applications of metal organic frameworks (MOFs) and polyanionic compounds (silicates, borates) as positive electrode materials have been investigated. MOFs with redox active metal centres have the potential for development as high capacity electrode materials with inherent structural stability and flexibility. A number of Prussian blue type analogues have been synthesised and Na inserted chemically. Electrochemical investigations of the insertion properties are underway. For the polyanionic compounds, Na analogues of established Li-ion insertion materials are investigated. The syntheses of many of these compounds have been completed and structural characterisation and property measurements are underway.

Relaxor ferroelectrics in the Ba-Sr-Ti-Nb-O and Sr-Zr-Ti-Nb-O systems (Whittle, Howard†): 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 or closely-related tungsten bronze type structures. Structural investigations were performed using a combination of synchrotron X-ray and neutron powder diffraction data as well as thermogravimetric analyses (TGA). Composition and temperature dependent phase transitions were determined in all systems. Ferroelectric properties were investigated for selected samples.

† Collaborators from outside the School of Chemistry

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Figure 1. Plot of the change in position and intensity of the 211 reflection during electrochemical operation of the cell. The change of the perovskite phase unit cell correlates nicely with the amount of lithium insertion (discharge) and extraction (charge).

Research in my group focuses on two major areas. Projects in Materials Chemistry aim to develop novel materials for, e.g., sustainable electrochemical storage applications. Chemistry Education research projects are designed to improve our understanding of how we best support student learning in a variety of formats.

ASSOCIATE PROFESSOR SIEGBERT SCHMID

Research in my group focuses on two major areas. Projects in Materials Chemistry aim to develop novel materials for, e.g., sustainable electrochemical storage applications. Chemistry Education research projects are designed to improve our understanding of how we best support student learning in a variety of formats.
ASSOCIATE PROFESSOR
MATTHEW TODD

We discover new ways to make molecules, either by studying reaction mechanisms or designing catalysts. Many of the molecules have uses as treatments for tropical diseases or as sensors for deployment in cells. We are devising new, open ways to carry out this research that allows anyone in the world to participate.

ORGANIC SYNTHESIS, CATALYSIS AND MEDICINAL CHEMISTRY

The Open Source Malaria Consortium: 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 contribute. 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 by groups 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. Despite there being no patents on our discovery it is being developed by a company for the international market.

We have extended this idea to open source drug discovery. With the Medicines for Malaria Venture, GlaxoSmithKline and a consortium of people who have spontaneously joined the project, we are prosecuting a hit-to-lead campaign in antimalarial drug discovery where all data and ideas are freely shared: The Open Source Malaria (OSM) Consortium. We have devised a technical platform applicable to any transparent, patent-free research endeavour. The OSM project is now working on a series of molecules with demonstrated in vivo efficacy in curing malaria. This research may demonstrate a new way to discover medicines, and was selected for one of three Wellcome Trust/Google/PLoS ASAP awards for its unique achievements and structure. We have recently started a related open source consortium for the discovery of new drugs for the treatment of tuberculosis.

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 new carbon-carbon bond forming processes such as those that generate chiral diamines, a class of compounds that is of central importance to both medicine and 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 an exciting and productive area for the group’s research.

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 behaviour.

References:

NOVEL LIQUIDS AND SOLVENTS

Ionic liquids (Jiang, Bryant, FitzGerald, Dolan, Adamson, Sherman, Atkin, Page, Chen, Murphy, Elbourne, Imberti, Watanabe): Our work on room-temperature ionic liquids (ILs) focuses on understanding how their unique physical and chemical characteristics arise from their nanoscale structure. Using neutron diffraction at the Rutherford Appleton Laboratory in the UK, together with X-ray scattering, we have found striking differences between ILs upon changing cation or anion.

The self-assembly of complex solutes like surfactants, lipids and block-copolymers is also sensitive to IL nanostructure. Although many ILs support amphiphilic self-assembly, they do not simply mimic water: Addition of simple molecular solutes like aliphatic alcohols leads to the formation of microemulsion-like fluids.

ILs form layers at a bulk interface, but these have been shown to retain vestiges of the bulk liquid nanostructure parallel to the macroscopic surface, which is important for understanding lubrication, electrochemistry, and heat transfer processes.

Deep eutectic solvents (Dolan, Tonini, Bryant, Atkin): Closely related to ILs, these are mixtures of salts and molecular species that form a stable liquid far below the melting point of either pure component. We have found that these liquids can exhibit nanostructure in bulk and at interfaces, and can also be solvents for amphiphilic self-assembly, thus heralding a new class of solvents for novel forms of soft matter.

Polymer nanocomposites (Wood, Atkin, McDonald): Inorganic nanoparticle/polymer hybrid materials have great promise for generating materials with new properties. Contrary to conventional wisdom, we have shown that covalently-bonded polymers are unlikely to lead to liquid nanocomposites, with both bulk and surface structure relying on excess polymer to sustain particle mobility needed for fluidity.

RESPONSIVE AMPHIPHILES

Photoresponsive systems (FitzGerald, Abe, Sakai, Akamatsu): Amphiphilic materials with photoreactive groups are a novel class of smart or responsive materials that can reversibly assemble and disassemble in response to light. Using small angle neutron scattering we have shown how micelle shape size and solubilisation capacity of photoisomerizable surfactants are affected by irradiation, and how similar results can be achieved using photoactive counterions in ionic surfactant systems.

pH-responsive systems (Liu): Using the simple device of hydrolysable counterions (phosphate, carbonate and oxalate), we have shown that the micelle and liquid crystal structure of cationic surfactant systems can be tuned to produce novel meshes and cubic phases. Adding calcium can yield mesoporous template structures reminiscent of biogenic materials.

Responsive co-oligomers (Lam, Gupta, Feeney, FitzGerald): Controlled free-radical (RAFT) polymerization allows us to prepare copolymers with exquisitely controlled architectures, and shorter block lengths than ever before. This brings copolymer self-assembly into the realm of conventional surfactants, but with the extensive library of vinyl monomers available to use. We have prepared libraries of amphiphilic block co-oligomers incorporating temperature- or pH-responsive monomers, and examined the structure and stability of micelles and lyotropic liquid crystal phases, generating dynamic materials with new and unexpected properties.
THEORETICAL AND COMPUTATIONAL NANOSCIENCE

Ligand-mediated interactions between nanoparticles (Geissler – U.C. Berkeley): Nanoparticles are appealing building blocks for creating new materials via solution-phase processes. Depending on the application, it can be desirable for the particles to be well dispersed or aggregated into structures with specific morphologies. Assessing and controlling the interaction between the particles, a key factor in their assembly and stability to random aggregation or sintering, are therefore important challenges.

Many nanoparticles are covered in ligand monolayers, which we have shown can undergo a temperature-dependent ordering transition in solution that is capable of switching the particle-particle interaction from repulsive to attractive. Recently, we have discovered that multiple distinct ordered states can exist – depending on the ligand surface coverage and the particle facet dimensions – that differ in how the ligands are packed together (Fig. 1). This can lead to non-linear changes in the thickness of the ligand shell, the critical temperature at which ordering occurs, and the interaction between the particles.

Our results add to a growing body of evidence that ligand-mediated interactions can exert a particularly strong influence on the assembly of faceted nanoparticles. Such control levers can be used to determine whether nanoparticles remain suspended in solution, randomly aggregate, or undergo assembly into large-scale ordered structures.

Assembly of nanorods for solar energy applications (Zhang, Latash, Phillips, Modestino – EPFL, Segalman – U.C. San Diego): 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. To this end, we are investigating how rod-shaped nanoparticles form ordered aggregates in solution and at interfaces with the goal of finding a robust way to assemble large ‘carpets’ of aligned nanorods (Fig. 2). This ARC-funded project involves the development of new simulation techniques and international collaboration with experimentalists who have used SAXS to study self-assembly in rod/polymer mixtures.

Figure 1. Alkyl ligands bound to the surface of a CdS nanoparticle can arrange themselves into distinct ordered states depending on the particle dimensions and the ligand surface coverage, which changes how the particles interact with one another in solution.

Figure 2. Rod-shaped nanoparticles can assemble into liquid-crystal-like aggregates in solution and at interfaces, which can potentially be used to print materials with anisotropic transport properties.

DR ASAPH WIDMER-COOPER

We use mathematical modelling and computer simulations to explain the behaviour of existing materials and to design new materials for solar energy capture, sensing, and optics. We are particularly interested in the dynamical properties of complex fluids and the beautiful structures that appear spontaneously in these systems through the self-assembly of molecular and colloidal components.


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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.

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Awarded for outstanding improvement in Chemistry performance between Junior and Intermediate Chemistry unit of study.

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Awarded on the basis of academic excellence and outstanding research potential to postgraduate scholars working in the field of Food Chemistry.

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

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Awarded for proficiency in both a Semester 1 and a Semester 2 Junior Chemistry unit.

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Awarded on the results of the Honours examination in the area of Organic Chemistry, provided that the student is of sufficient merit.

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

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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.

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- Mr Andrew Giltrap
- Mr Jordan D'Arcy
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Three scholarships have been awarded for proficiency in both Semester 1 and Semester 2 Senior Chemistry units of study by a student proceeding to Honours in Chemistry.
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Awarded annually on the recommendation of the Head of the School of Chemistry for outstanding performance in Senior Chemistry by a student proceeding on to an Honours year in Theoretical Chemistry.
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Awarded for proficiency in both Semester 1 and Semester 2 Senior Chemistry units of study by a student proceeding to Honours in the area of Organic Chemistry.
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Awarded for the most proficient female student who has completed Chemistry Honours.
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Established in 2002 from matching contributions by the Surface Coatings Association Australia and the University, the purpose of this scholarship is to foster the further advancement of education in coating fields. The student must be enrolled in the MSc or PhD degree within the School of Chemistry and working in the area of surface coatings (including pigments, polymers, corrosion, weathering, adhesion and methods of manufacture).

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The following students had their degrees awarded in 2015:-

Mr Julian Burbidge
Synthetic studies towards lycoranine A
Research supervisor:  Associate Professor Christopher McErlean

Mr Isaac Carney
Development and application of fluorescent iron probes
Research supervisors:  Dr Elizabeth New and Professor Trevor Hambley

Mr Jonathan Chung
Synthesis and evaluation of gallinamide A analogues as novel antimalarial agents
Research supervisor:  Professor Richard Payne

Mr Andrew Counsell
Spectroscopic and crystallographic characterisation of propargylic tetraazamacrocycles
Research supervisor:  Associate Professor Peter Rutledge
Auxiliary supervisor:  Associate Professor Mat Todd

Mr Isaac Freelander
N-benzylindole-2-carboxamides and analogues as potential neurotherapeutics targeting the translocator protein (TSPO)
Research supervisor:  Professor Michael Kassiou

Ms Haihui Jiang
Amphiphilic self-assembly in protic ionic liquids and their mixtures
Research supervisor:  Professor Greg Warr

Ms Haishui Jiang
Amphiphilic self-assembly in protic ionic liquids and their mixtures
Research supervisor:  Professor Greg Warr

Mr Henry Jiang
Incorporation of the redox-active ligands TCNE and TCNQ into mental-organic frameworks
Research supervisor:  Dr Deanna D’Alessandro
Auxiliary supervisor:  Professor Timothy Schmidt

Mr Lachlan Lindoy
Path integral formalisms beyond the primitive approximation
Research supervisor:  Associate Professor Meredith Jordan

Mr Gabriel Murphy
The crystal chemistry of AUO, oxides
Research supervisor:  Professor Brendan Kennedy

Ms Lisa Player
Exploring the heterogeneous solvation environment of novel bromozincate ionic liquids
Research supervisor:  Associate Professor Tony Masters
Auxiliary supervisor:  Professor Thomas Maschmeyer

Ms Keyun Shou
Self-assembled monolayers on silicon based on halogen bonding
Research supervisor:  Associate Professor Chiara Neto

Mr Christopher Tangvisethpat
A multi-residue dried blood spot method for doping control using aleternative blood collection platforms
Research supervisor:  Dr Adrian George

Ms Emma Watson
Dihydrosansanmycin analogues as novel anti-tubercular agents
Research supervisor:  Professor Richard Payne

Ms Laura White
Investigating structure-activity relationships of small molecule non-peptidic probes of the oxytocin-vasopressin receptor system
Research supervisor:  Professor Michael Kassiou

Mr Jared Wood
Nanoparticle organic hybrid materials: The preparation, characterization and self-assembly of these unusual composites
Research supervisor:  Professor Greg Warr
Ms Katrina Zenere
Spin crossover, functionality and guest exchange of triazole-based two-dimensional Hofmann-type framework materials
Research supervisor: Dr Suzanne Neville
Auxiliary supervisor: Professor Cameron Kepert

Mr Malcolm Ramsay
The role of molecular shape on the properties of the condensed phase: A simulation study
Research supervisor: Professor Peter Harrowell

Mr Liam Scarratt
Fabrication of robust superhydrophobic surfaces through spontaneous wrinkling
Research supervisor: Associate Professor Chiara Neto
Auxiliary supervisor: Associate Professor Brian Hawkett

Ms Elisabeth Tondl
Towards the synthesis and testing of model tumour-activated prodrugs for prostate cancer
Research supervisor: Professor Trevor Hambley

Mr Sam Peppou-Chapman
Blue fluorescence on the surface of nanodiamond
Research supervisor: Dr Mohammad Choucair

Ms Cecile Elgindy
Studies towards the total synthesis of hinckdentine A
Research supervisor: Associate Professor Christopher McErlane

Mr Alexander Horry
Towards a platinum (IV) - PSMA substrate complex to enhance tumour selectivity
Research supervisor: Professor Trevor Hambley

Mr Thomas MacDonald
Development of routes to access and functionalise [1,2,4]triazolo[4,3-α]pyrazine amides as new antimalarial compounds
Research supervisor: Associate Professor Mat Todd
Auxiliary supervisor: Associate Professor Peter Rutledge

Mr Pierre Naeyaert
Synthesis, structure and electrochemistry of Mn−Na$_4$Ti$_5$O$_{12}$: A new anode material for sodium-ion batteries
Research supervisor: Associate Professor Chris Ling

Ms Joanna Ubels
Synthesis of novel triazolopyrazines as candidate antimalarials
Research supervisor: Associate Professor Mat Todd
Auxiliary supervisor: Associate Professor Peter Rutledge

Mr James O’Brien-Brown
Design and synthesis of novel P2X$_7$ receptor antagonists for the treatment of inflammatory and neurodegenerative diseases
Research supervisor: Professor Michael Kassiou

Ms Samantha Zaiter
Discrete and polymeric spin crossover materials
Research supervisor: Dr Suzanne Neville
Auxiliary supervisor: Professor Cameron Kepert

Mr Eddie Zwicker
Pyrophosphate recognition by linear peptide based receptors in aqueous media
Research supervisor: Professor Kate Jolliffe
BACHELOR OF SCIENCE (ADVANCED MATHEMATICS) WITH HONOURS
The following student had his degree awarded in 2015:-

Mr Ignazio Cristina
Understanding change transfer in coordination polymers
Research supervisor: Dr Deanna D'Alessandro
Auxiliary supervisor: Professor Jeffrey Reimers

MASTER OF SCIENCE
The following student had her degree awarded in 2015:-

Ms Ayesha Hussain
Iron promoted allylic amination of unactivated alkenes
Research supervisor: Associate Professor Peter Rutledge
Auxiliary supervisor: Professor Richard Payne

DOCTOR OF PHILOSOPHY
The following students had their degrees awarded in 2015:-

Dr Josie Auckett
Structural and physical studies of oxide ionic-conductive brownmillerite single crystals
Research supervisor: Associate Professor Chris Ling
Auxiliary supervisor: Professor Brendan Kennedy

Dr Alessio Caretto (Cotutelle student)
Green transformations of bio-based chemicals
Research supervisor: Professor Thomas Maschmeyer
Associate supervisor: Associate Professor Tony Masters
Research supervisors from the partner institution: Associate Professor Alvise Perosa and Professor Maurizio Selva (Ca' Foscari University of Venice)

Dr MD Sadrul Ahsan Chowdhury
Computational studies of structure and dynamics in amorphous materials
Research supervisor: Professor Peter Harrowell
Auxiliary supervisor: Dr Toby Hudson

Dr Chun Croucher
On probing the mechanisms of thermal expansion and the effects of bare metal sites on the hydrogen storage properties of metal-organic frameworks
Research supervisor: Professor Cameron Kepert
Auxiliary supervisor: Professor Brendan Kennedy

Dr Manuel Ghezzi
Functional surface micropatterns by dewetting of thin polymer films
Research supervisor: Associate Professor Chiara Neto
Auxiliary supervisor: Dr Stuart Thickett

Dr Bligh Gibson
Excited state interactions of isolated molecules
Research supervisor: Professor Scott Kable
Auxiliary supervisor: Professor Tim Schmidt

Dr Xiaoyun Gui
Towards the specific targeting of regions of solid tumours remote to the vasculature
Research supervisor: Professor Trevor Hambley
Auxiliary supervisor: Associate Professor Lou Rendina

Dr Byung Kim
Development of multiple fluorescent tumour spheroid models to investigate the use of transition metal complexes as hypoxia-activated prodrugs
Research supervisor: Professor Trevor Hambley
Auxiliary supervisor: Dr Nicole Bryce

Dr Stephen Kolmann
Accurate studies of weakly bound systems
Research supervisor: Associate Professor Meredith Jordan
Auxiliary supervisor: Professor Cameron Kepert
Dr Anthony Lo  
*Novel polyamide amidine anthraquinone platinum(II) complexes for enhancing DNA binding and tumour penetration*  
Research supervisor: Professor Trevor Hambley  
Auxiliary supervisor: Associate Professor Mat Todd

Dr Michael Murphy  
*On the gas sorption, thermal expansion and magneto-structural correlations in coordination frameworks*  
Research supervisor: Professor Cameron Kepert  
Auxiliary supervisor: Dr Deanna D'Alessandro

Dr Peter Phung  
*Biofuels: Method for improving cold-flow characteristics of biodiesel. Non-catalytic hydrolysis of carboxymethylcellulose in subcritical water and lignin model compound syntheses and screening*  
Research supervisor: Associate Professor Tony Masters  
Auxiliary supervisor: Professor Thomas Maschmeyer

Dr Cheuk Ka Poon  
*Preparation of sterically stabilised polymeric nanoparticles as microrna delivery vectors by surfactant-free raft emulsion polymerisation and post-modification*  
Research supervisor: Associate Professor Brian Hawkett  
Auxiliary supervisor: Professor Sébastien Perrier

Dr Gajan Santhakumar  
*Studies towards the total synthesis of non-ribosomal peptide natural products*  
Research supervisor: Professor Richard Payne  
Auxiliary supervisor: Professor Kate Jolliffe

Dr Jessica Stanley (Cotutelle student)  
*Novel applications of catalysis for green and sustainable chemistry*  
Research supervisor: Professor Thomas Maschmeyer  
Associate supervisor: Associate Professor Tony Masters  
Research supervisors from the partner institution: Associate Professor Alvise Perosa and Professor Maurizio Selva (Ca' Foscari University of Venice)

Dr Jessica Tom  
*Application of controlled/"living" radical polymerisation techniques in the preparation of polymer hybrid materials*  
Research supervisors: Associate Professor Chiara Neto and Associate Professor Brian Hawkett  
Auxiliary supervisor: Professor Sébastien Perrier