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Front cover: Portrait of A/Prof. Ruth Gall (1923-2017), the first woman to Head the School of Chemistry at the University of Sydney, painted by local artist Dr Kate Gradwell.

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.

WELCOME

HEAD OF SCHOOL

Professor Phil Gale
Head of School
School of Chemistry

2017 saw the School of Chemistry sustain and strengthen its leadership position in research and teaching in Australia and internationally. The University of Sydney remained in the top 50 Universities for Chemistry in the QS rankings and given the strong competition from across the globe, this was a great achievement. 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 2017, members of the School received over $4.2M in new research funding, leading to a total of 19 Discovery Grants, 2 Future Fellowships, 2 other Fellowships, and 5 Linkage Grant from the Australian Research Council, totaling (with other grants) $8.1M in competitive research funding. In 2017 the School maintained its strong publication record, collectively producing 1 book chapter and 249 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 2017 include the RJW Le Fèvre Memorial Prize to A/Prof Deanna D'Alessandro; Dr Ivan Kassal was the recipient of the Tall Poppy Award; A/Prof Liz New was a finalist in the 3M Eureka Prize for emerging leader in science; Prof Kate Jolliffe was awarded A.J. Birch Medal; Mr Phil Karpati was the global winner of the 2017 Undergraduate Awards - Phil was also awarded a 2017 Westpac Future Leaders scholarship; and the RACI Cornforth Medal for the best PhD thesis in Australia went to Ms Amandeep Kaur.

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 100 higher degree research students in the School in 2017 there were 40 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 Phil Gale
Head of School

ASSOCIATE PROFESSOR RON CLARKE

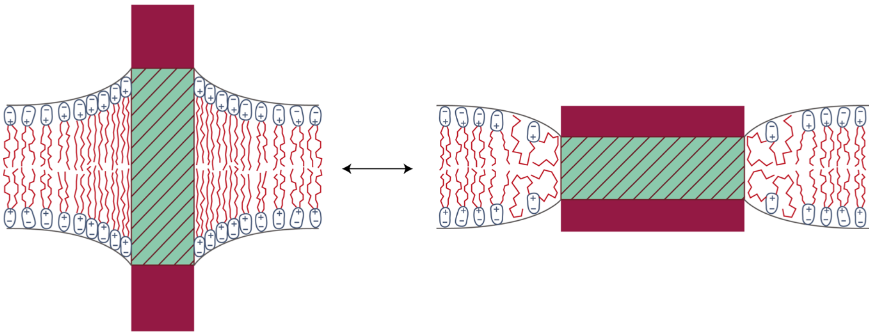
The focus of our research is on the function of ion-transporting membrane proteins, without which no cellular life forms are imaginable. We are interested in the mechanisms of these enzymes, their physiological regulation by their membrane environment and their chemical evolution. Our major object of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

BIOPHYSICAL CHEMISTRY OF MEMBRANES

Mechanism and regulation of the Na^+,K^+-ATPase *(Cornelius[1], Allen[2], Rasmussen[3]):* 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.



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[1] *University of Aarhus, Denmark*

[2] *RMIT University, Melbourne*

[3] *Royal North Shore Hospital, Sydney*

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.

FUNCTIONAL ORGANIC MOLECULES

Porphyrins and their properties *(Sintic, Brooks, Canfield, Reimers, Roberts, Perrier):* Using functionalisation processes developed in our laboratory, regioselective synthesis of bio-inspired oligoporphyrin helices was further developed. Molecular modeling showed that these structures are akin to RNA. There are many possible uses of this new class of compounds. New triazole–linked porphyrin–polymer dendritic compounds were synthesized for construction of porphyrin arrays for use in light harvesting and in catalysis.

Self-assembled silica microwires *(Naqshbandi, Ma, Lindoy, Canning, Cook, Peng,* Huyang, Kristensen,* Martelli*):* A new platform for optical sensing was developed by room temperature self-assembly of silica nanoparticles into microwires that have been grown to 13 cm in length. These wires are remarkably uniform and hundreds are produced at a time without the need for further processing. Organic materials including porphyrins and enzymes were incorporated into the microwires and self-assembled micro-slabs. Work is ongoing looking at new composites and exploring new possibilities for functional devices.

Porphyrins on surfaces *(Reimers, Indusegaram, Tong, Rehn, Kafi,* Naqshbandi, Choucair, Elemans*):* A conductive network of crosslinked carbon nanotube/cytochrome *c* on graphene surfaces were constructed. Polymorphism in porphyrin monolayers was also explored and the relation 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 formation 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 properties 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 monodispersed Al^{3+}-doped SiO_2 nanoparticles (20-30 nm) possessing interparticle mesospaces suitable for incorporating Pt 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 compounds 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 system 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 lithocholic acid were completed.

ASSOCIATE PROFESSOR DEANNA D'ALESSANDRO

Our research spans the areas of inorganic chemistry, physical chemistry and materials science and focuses on the development of functional inorganic materials which exhibit novel optical and electronic phenomena.

FUNCTIONAL INORGANIC MATERIALS

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

Electroactive MOFs *(Murase, Ding, Leong, Sherman):* Our work has involved the design and synthesis of MOFs which exhibit the highly sought after property of redox activity and ultimately, electronic conductivity (Figure 2). 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.

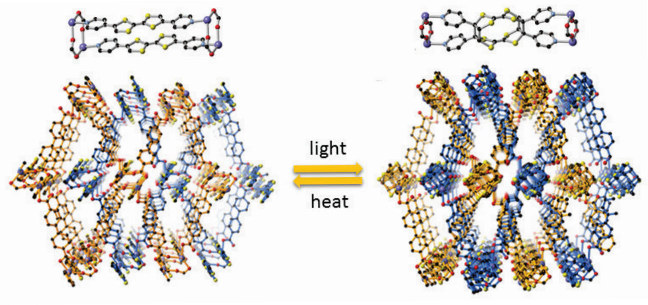


Figure 1: The novel MOF incorporating cofacially-aligned tetrathiafulvalene units. Light-irradiation induces cyclisation of the ligands and crystal 'breathing'.

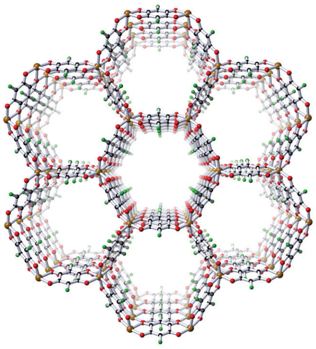


Figure 2: A graphitic honeycomb MOF that displays intrinsic conductivity due to mixed valency

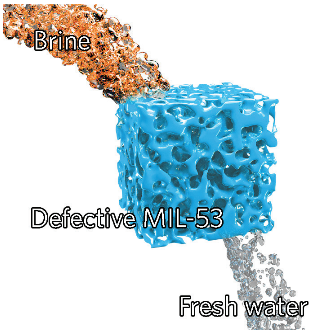


Figure 3: Schematic of a MOF desalination membrane

The interplay between conductivity and magnetism in microporous materials *(Doheny, Ding, Kepert):* In collaboration with Professor Cameron Kepert, we have synthesised novel triselenafulvalene ligands and have incorporated these into new charge transfer framework structures. 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 *(Solomon, Kepert):* The development of more efficient processes for CO_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 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_2 framework interactions which give rise to this activity. We are also currently integrating MOFs into membranes for desalination in collaboration with Chemical Engineering at UNSW (Figure 3).

DR ADRIAN GEORGE

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

SYNTHESIS AND ANALYSIS

Detection of 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, β2-agonists, hormones, diuretics, stimulants, narcotics, cannibimimetics, β-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. Recently, very pure samples of some synthetic drugs, such as methylamphetamine, have been seized. This makes chemical profiling by use of the impurities more difficult. In these cases, profiling is based on the use of isotope ratio mass spectrometry.

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 has the potential to overcome many of the toxic side effects of existing drugs and allow higher doses to be used. Better tumour penetration will enable the destruction of cells that presently evade treatment and contribute to resistance.

MEDICINAL INORGANIC CHEMISTRY

Monitoring the penetration and effectiveness of anticancer drugs in solid tumour models *(Chen, Glenister, Renfrew):* A limiting factor in the effectiveness of current anti-cancer treatments is the inability of the drug to penetrate throughout the entire tumour at concentrations sufficient to kill all cancer cells. The aim of this project is to develop and use techniques to study anti-cancer drug penetration and the effect of those drugs on cell status and viability in cell monolayer and 3-dimensional cellular models of solid tumours (spheroids). In Figure 1 are elemental maps showing platinum and zinc distributions in tumour spheroids, that have been dosed and incubated with model platinum based anti-cancer drugs, were generated using synchrotron generated X-ray radiation.

Targeted delivery of metal complexes for anticancer applications *(Chen, Glenister, Lim, Renfrew, Simone*, Tondl):* 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) and cobalt(III) complexes.

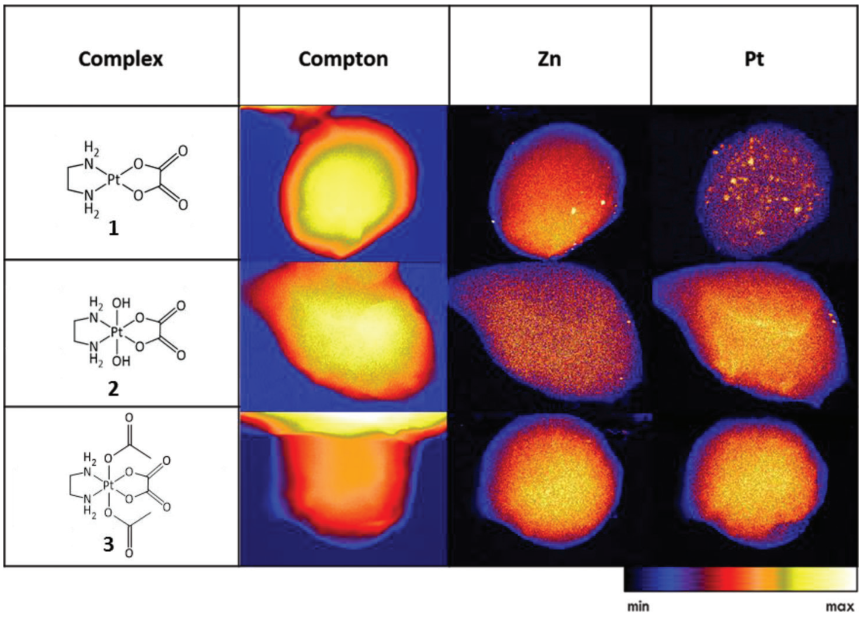


Figure 1: XRF elemental maps of whole DLD-1 spheroids dosed with cis-platinum(II) (1) and cis-platinum(IV) (2 and 3) complexes at 50 µM and incubated for 6 h, showing Zn, Pt and scattered X-rays. Maximal densities are shown.

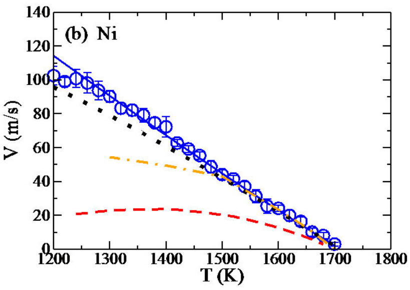
Work was continued into the stabilisation of platinum(IV) compounds and their functionalisation with targeting groups. New examples of a novel series of platinum(IV) complexes that generate a positively charged platinum(II) complex on reduction were sought and synthetic strategies for adding targeting groups such as the PSMA substrate were investigated. The intracellular accumulation and reduction of platinum(IV) complexes was studied using XANES spectroscopy and X-ray fluorescence microscopy. 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 PETER R HARROWELL

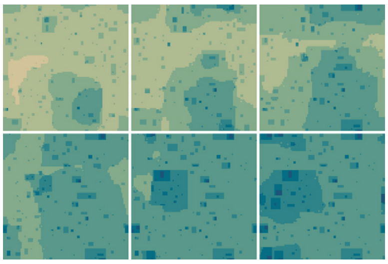
I am interested in understanding the structure, dynamics and phase transitions of liquids and solids. Topics include understanding the relation between glassy solids and viscous liquids, the factors that control how fast a liquid can freeze and how rigidity comes to be. My tools are model building, computer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

THEORETICAL CHEMISTRY

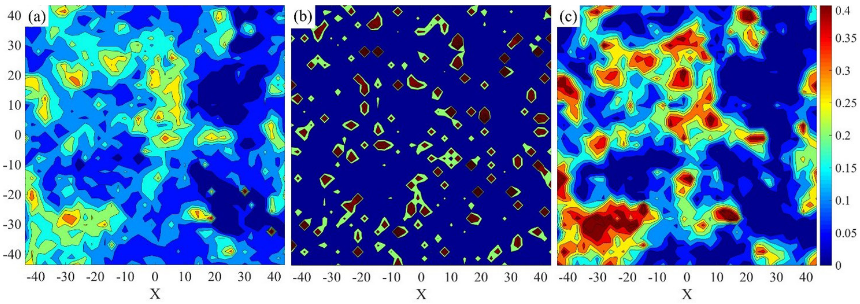
Ultra fast crystal growth of pure metals *(Sun):* We typically associate activated dynamics with processes occurring a liquid such as diffusion and chemical reactions. It is remarkable, therefore, that crystal growth of pure metals occurs with no sign of thermal activation at all. Using computer simulations we have established that the extraordinary high growth rates (~ 100m/s) of these crystals is a result of a highly effective pre-ordering of the liquid in advance of the interface, an effect only made visible by applying computer methods developed to study relaxation in glass-forming liquids.



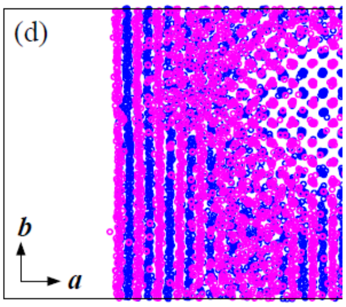
Kinetics of dissolution of an amorphous solid *(Douglass):* The rate of dissolution of amorphous solids is an important aspect to the delivery a number of drugs. In this study we developed a simple model of the glassy solid that permitted efficient simulations while providing an accurate representation of the cooperative kinetics of relaxation. We report how the stability of the glass surface determined the dissolution rate and explore the possibility of using solvent etching to visualize heterogeneous mobilities of the solid.



The role of dynamic reversals in the slow dynamics close to the glass transition *(Sun):* The growing heterogeneity of relaxation kinetics observed in a supercooled liquid on cooling is shown to arise from the spatial heterogeneity of the likelihood of reversal of reorganization rather than from the probability of the reorganization itself. Computer simulations on a model glass forming alloy reveal that the spatial distribution of relaxation kinetics (left panel) is not described by the spatial distribution of the probability of reorganizations (centre panel) but rather by the distribution of irreversibility (right panel).



Chemical ordering and crystal growth at the liquid surface *(Tang, UNSW):* While a good glass former, $Cu_{50}Zr_{50}$ shows no evidence of surface enhancement of crystallization, $Ni_{50}Al_{50}$ exhibits an increased rate of crystallization due to heterogeneous nucleation at the free liquid surface. The difference in the compositional fluctuations at the interface is proposed as the explanation of the distinction between the two alloys.



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.

POLYMER AND COMPOSITE COLLOIDS

Key functional additives in paint technology *(Neto, Nguyen, Zhu, Davey, 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 proved 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 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 amount of pigment 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 making 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, S. 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. 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.

Polymer coated zero valent iron particles *(Pham, Nguyen, Huynh, Rider, Charles):* Funded by DSTG, this project extends our particle coating technology to larger (micron sized) and reactive particles.

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, Christie, Lindsay):* 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, Sabouri, 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.

Figure 1: TiO_2 particles encapsulated by polymer

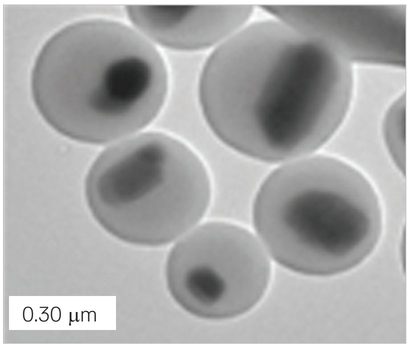


Figure 2: Spikes in EMIM NtF2-based ionic liquid ferrofluid

DR TOBY HUDSON

Predicting and understanding the structures and phase behaviour of liquids, crystals, and everything in between.

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.

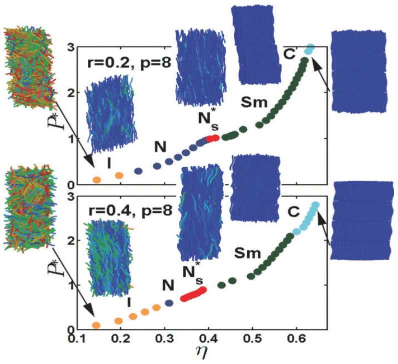


Figure 1. Equations of state for helical particles, including the screw-like phase in red

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?

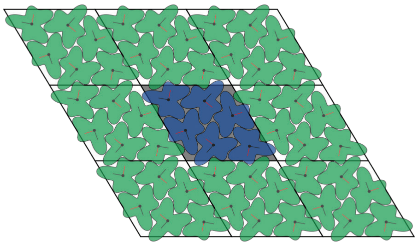


Figure 2. A dense packing of an irregular particle with the rare p6 symmetry

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).

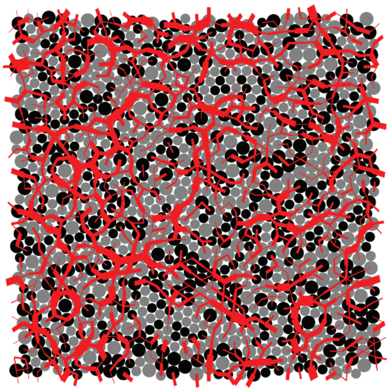


Figure 3. The force network and stress correlations in an inherent state of a binary glass

PROFESSOR KATRINA JOLLIFFE

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 ions and, in some cases, transporting these across a lipid membrane.

ORGANIC SYNTHESIS AND SUPRAMOLECULAR CHEMISTRY

Novel anion receptors and transporters *(Dergham, 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 we have shown that some of these can transport sulfate ions across a bilayer membrane.

The Jolliffe group

Efficient synthesis of natural and novel cyclic peptides *(Falvey, Glen*):* 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.

New fluorophores for use in molecular imaging *(Leslie, New):* In collaboration with Dr Liz New we are developing novel fluorophores that can be incorporated into fluorescent probes for a range of analytes (anions, cations and small molecules). We have established that the fluorescence of naphthalimide derivatives can be modulated in a predictable way through the incorporation of additional substituents on the aromatic skeleton and have substantially increased the wavelength range at which these dyes are able to fluoresce.

ASSOCIATE PROFESSOR MEREDITH JORDAN

I use theoretical and computational chemistry to examine the interactions within and between molecules in order to understand chemical reactivity and the relationship between structure and function in chemistry, biology and materials science.

INTERMOLECULAR INTERACTIONS

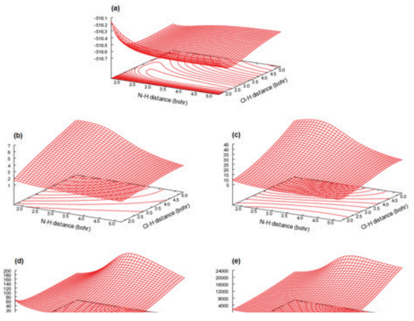
Potential energy surfaces: Molecular potential energy surfaces (PES) describe how the energy of a molecule changes as its atoms move. We have developed new interpolation techniques for constructing PES based on *ab initio* quantum chemical calculations.. These are contained in our freely available *Grow computer package*.

Hydrogen storage materials *(Kolmann, D'Arcy):* We have used *Grow* to develop a reduced-dimensional model to mimic 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 H_2 binding enthalpies and vibrationally averaged (ground state) structures. They demonstrate that the 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 H_2 molecules.

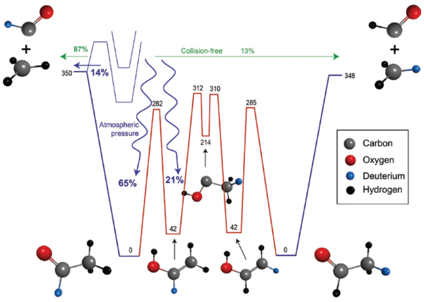
Molecular property surfaces *(Morris):* Our interpolation techniques have been used to describe molecular dipole moment and polarizability surfaces. These surfaces and the PES have then been used to calculate rovibrational intensities and demonstrate that the effects of an external electric field (a 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.



Above: (a) Potential Energy and Molecular Property Surfaces: (b) $|\mu_z|$, (c) $|\Theta_{zz}|$, (d) $|\alpha_{zz}|$, and (e), $|C_{zz,zz}|$for $ClH{:}NH_3$

We have also investigated triple fragmentation and photo-chemically-induced isomerization using both theory and experiment. We have shown that, under atmospheric conditions, acetaldehyde, CH_3CHO, can isomerise to vinyl alcohol, $CH_2{=}CHOH$, 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.



Above: A schematic showing energies (kJ/mol) and important structures on the CH_3CDO 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.

Computational drug design *(Hunter (UNSW)):* Fluorinated analogues of γ-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.

DR IVAN KASSAL

Energy and charge transport underpin photosynthesis, solar cells, combustion, corrosion, batteries, and molecular electronics. We are developing cutting-edge theoretical tools—including the use of quantum computers—to better simulate these processes and design superior devices.

CHARGE AND ENERGY TRANSPORT

Fundamental processes: The transfer of charges (or excitation energy) from one molecule to another—perhaps the simplest chemical reaction—is a fundamentally quantum-mechanical process. However, because a fully quantum treatment of charge transport in disordered materials can be computationally prohibitive, many models use purely classical concepts, such as molecule-to-molecule charge hopping. Classical simulations can fail dramatically, which is why we are working on new quantum theories to treat charge and energy transport without incurring an excessive computational cost. For example, we recently developed a theory for the transfer of delocalised charges, explaining how charges hop if they are—as is often the case—smeared out over several molecules.

Photosynthesis: Quantum coherence is usually thought to be too fragile to persist in warm and noisy environments such as the light-harvesting units of photosynthetic organisms. After the discovery of coherent signals in spectroscopic studies of photosynthesis, debate raged about whether coherence could enhance the efficiency light harvesting. We have shown how quantum effects observed in laser experiments translate to biological function in sunlight and, in doing so, we discovered the most significant coherence-related enhancement of energy transport ever found in a photosynthetic complex. We also identified two coherent mechanisms that could be used for improving artificial light harvesting and, with experimental colleagues, have already demonstrated one of them—the other is on the way.

Organic electronics: Organic semiconductors can be made into organic light emitting diodes (OLEDs) for displays and lighting, organic photovoltaics (OPVs) that promise truly green energy, and organic field-effect transistors (OFETs) for general-purpose flexible electronics. We are developing new theories to describe charge and energy motion in organic electronics, especially OPVs, so that rational design can replace the current trial-and-error approach. We recently explained why the electron and the hole separate *at all* to form an electric current: their Coulomb attraction was previously thought to be insurmountable, but we showed they can overcome it using entropy and disorder.

QUANTUM COMPUTER FOR CHEMISTRY

We have been at the forefront of applying quantum computation to problems in chemistry ever since Ivan's PhD, which was the first on the topic. We have shown that quantum computers could solve chemical problems much faster than conventional computers, and have developed a complete suite of quantum-computer software for chemistry, for everything from reaction dynamics to molecular properties. Today, chemistry is seen as a killer app for quantum computers, with chemical applications targeted by all the major quantum computing companies.

We have strong collaborations with experimentalists, including the first experimental chemical calculation on a quantum computer, in 2010. We are currently working on the first quantum-computer simulation of a chemical reaction, a charge-transfer process.

For details, visit www.kassal.group

Kassal Group 2017

PROFESSOR MICHAEL KASSIOU

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

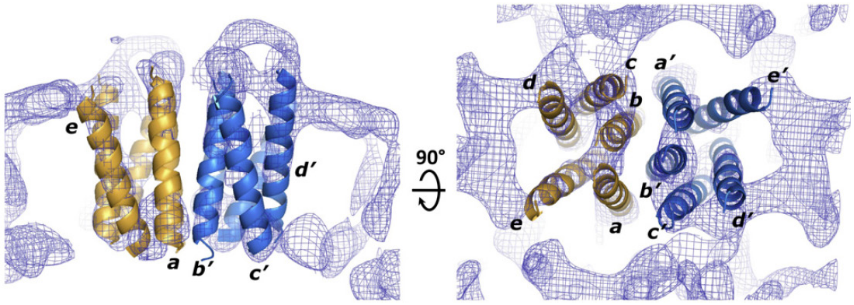
DRUG DISCOVERY/MEDICINAL CHEMISTRY

Immunomodulation in the treatment and diagnosis of CNS disease *(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 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-1β (IL-1β), and tumour necrosis factor-a (TNF-α) is increasingly recognised as a potential cause of depression. The purinergic P2X$_7$ receptor modulates the maturation and release of cytokines such as IL-1β 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)



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 α7 nicotinic receptor subtype is particularly important in the potential treatment schizophrenia. We have developed structure-activity relationships strategies of the following small molecules in order to understand the motifs responsible for conferring α7 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 a novel series of trishomocubanes of the type 4-azahexacyclo[5.4.1.0^{2,6}.0^{3,10}.0^{5,9}.0^{8,11}] dodecane which display high affinity for sigma-2 and sigma-1 receptor subtypes respectively. These molecules have also been shown to modulate cocaine induced behaviours. These lead compounds provide the basis for further refinement of the binding and functional activity of this class.

PROFESSOR BRENDAN KENNEDY

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.

SOLID STATE AND MATERIALS CHEMISTRY

Defects and phase transitions

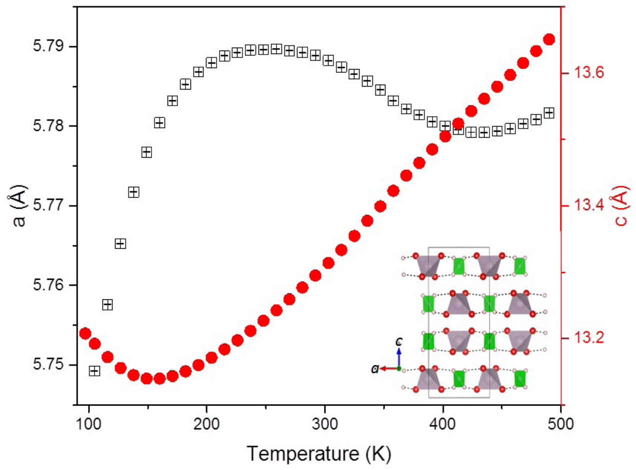
The perovskite $NaTaO_3$ shows promise as a photocatalyst for splitting water into H_2 and O_2. Cation doping is a powerful way to tune the band gap in perovskites and hence enhance the photocatalytic response, consequently efforts are being directed to understanding the correlation between the changes 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 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 $SrTaO_2N$ 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.

Structural transformations in uranium oxides

In-situ Synchrotron X-ray and Neutron Diffraction methods have been used to study the unusual phase transition behaviour of $SrUO_4$. At high temperatures and under oxidizing conditions the stable form, stoichiometric β-$SrUO_4$, contains UO_6 groups. Under mildly reducing conditions an oxygen deficient rhombohedral structure α-$SrUO_{4-x}$ forms in which oxygen vacancies are critical to the stability of the 8-coordinate UO_8 moieties. Treating α-$SrUO_{4-x}$ with H_2 at high temperatures induces a reversible phase transformation associated with the ordering of oxygen defects resulting in a lowering of crystallographic symmetry to give a triclinic polymorph, δ-$SrUO_{4-x}$. A strong reducing atmosphere is required to generate a critical amount of oxygen defects in α-$SrUO_{4-x}$ to enable the transformation to δ-$SrUO_{4-x}$ but once formed the transformation between these two phases can be induced by thermal cycling. Entropy changes associated with the temperature dependent short-range ordering of the reduced U species important in this transformation.

Structural trends in ABO_4 scheelite type oxides (B = Tc, Re, Ru, Os)

Re is often studied as a non-radioactive analogue to Tc, given their similar range of oxidation states and ionic radii resulting in similar chemical behaviour. Evidence is emerging that this may not be the case for solid state materials. The $AReO_4$ oxides were studied in order to allow for comparison with the analogous pertechnetates. As the size of the *A* site cation (Na, K, Rb, Cs, Tl, Ag, NH_4) increases the symmetry decreases from tetragonal to orthorhombic and this can reversed by heating the samples, the exception being $TIReO_4$ that exhibits an *unusual* reentrant phase transition involving a monoclinic structure. The ammonium salts $NH4BO_4$ (B = Tc, Re) exhibit unusual thermal expansion behaviour associated with hydrogen bonding. This work is being extended to include the magentic Ru and Os systems.



PROFESSOR CAMERON KEPERT

Our research focuses on the incorporation of multiple chemical and physical functions into molecular frameworks to yield materials with new, emergent properties.

MOLECULAR FRAMEWORK MATERIALS

Nanoporous molecular frameworks *(Southon, Ragon, Keene, Duyker, Chen, Murphy, Barkhordarian, Ogilvie, Zenere, Windsor, 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 H_2, CH_4, CO_2 and O_2. 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, Windsor, Diwa, Mullaney, Sciortino, Kirk, Klein, Price, Goux-Capes, Grünwald, Doheny, Hill, Southon, Halder, Murray, Moubaraki, 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.

The Kepert group

DR GIRISH LAKHWANI

Our research in the School of Chemistry underpins various research projects within the ARC Centre of Excellence in Exciton Science and beyond. The board area of our research overlaps the fields of physical chemistry, chemical physics and organic electronics. Our key focus is on developing spectroscopic methods to study optical and electronic properties of novel nanoscale semiconductor materials for solar energy harvesting, polarisation switching and polariton lasing.

Fluorescence blinking in quantum dots *(collaboration with Dr Akshay Rao, University of Cambridge):* The realisation of any opto-electronic thin film devices or technologies requires control over excitons at a nanoscale. In our group, we use single molecule spectroscopy to study photophysical processes at a single molecule level, which are otherwise obscured by conventional measurements that ensemble average optical properties of a heterogeneous distribution of molecules. Here we report stochastic fluorescence blinking in near infrared emitting (NIR) emitting of individual PbS core and PbS/CdS core shell quantum dots (Fig. 1). Fluorescence blinking is a reversible process that causes fluorescence to appear (on) and disappear (off) intermittently, at timescales of a few ms to seconds. We observe that PbS dots display longer off times compared to PbS/CdS core shell dots. We conclude that longer off times are a result of Auger recombination and reversible exciton diffusion between singlet energy levels and a large density of dark surface defect states. The distribution of defect states in core shell dots is relatively narrow, hence the on and off times are of similar time scales.

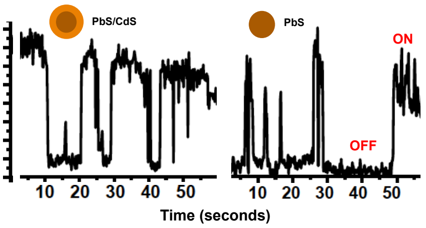


Fig 1. Single molecule fluorescence blinking from (left) PbS/CdS core-shell and (b) PbS quantum dots.

Polarisation sensitive fluorescence decay *(collaboration with A/Prof Tak Kee, University of Adelaide, Dr Stavros Athanasopoulos, University of Madrid and Dr Markus Müllner, USyd):* Structural disorder in molecular assemblies has a huge impact on the function of a wide variety of organic optoelectronic devices. Here, we use transient absorbance spectroscopy to demonstrate that fluorescence in donor-acceptor based copolymer aggregates follows different decay pathways when photoexcited by left and right handed circularly polarised light (CPL).

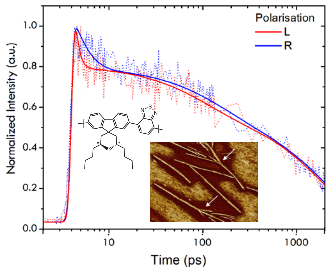


Fig 2. Fluorescence decay monitored at 530 nm for PFBT copolymer fibres (inset) for left and right CPL excitations at λex = 440 nm.

Comparing the two cases, we notice that virtually 20% of fluorescence intensity is lost within 5 picoseconds when excited with left and right circularly polarized light severely limiting the utility of these materials as ultrafast polarization switches. We demonstrate that the CPL sensitive rate of fluorescence decay emerges due to localization of photoexcitations at the disordered edges of polymer aggregates. Our findings open up new opportunities for sensitively exploring the links between intermolecular coupling and photophysical properties, crucial for the performance of a wide range of organic electronic devices.

Chiroptical phenomena in self-assembled perylene nanofibres *(collaboration with Prof Pall Thordarson, UNSW and Dr Markus Müllner, USyd):* The performance of organic optoelectronic devices is heavily dependent on the molecular packing and nanoscale morphology of molecular aggregates. In this work, we used Circular Dichroism (CD) and Magnetic Circular Dichroism (MCD) spectroscopy to study chiral perylenes both as isolated molecules and self-assembled helical nanofibres. By altering the size and helicity of the supramolecular nanostructures, we confirmed that while CD is sensitive to exciton coupling and long-range order, the MCD (also referred as Faraday Rotation) is a unique molecular property. The observed MCD is B-type, which is characteristically found in low symmetry systems. We find that the insensitivity of MCD to exciton coupling makes it a unique probe to study molecular photophysics decoupled from system-bath interactions (such as interactions with the solvent or a solid-state matrix) in complex supramolecular architectures.

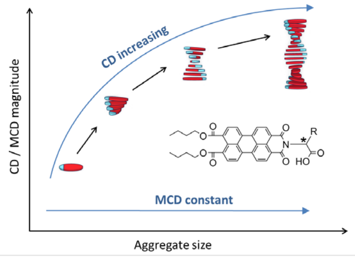
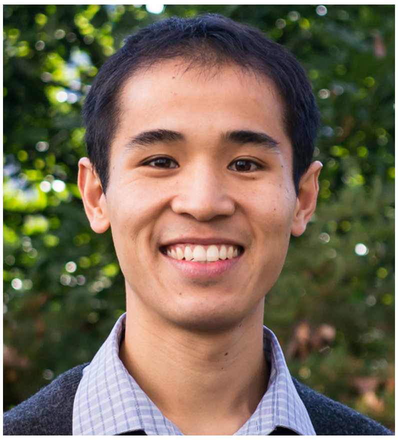


Fig 3. CD and MCD as a function of size of a helical supramolecular perylene aggregates.



DR YU HENG LAU

We combine chemical and biological synthetic methods, re-engineering macromolecules found in nature to create new medicines, materials and catalysts. Our research involves a mix of organic chemistry, synthetic biology and protein engineering.

CHEMICAL AND SYNTHETIC BIOLOGY

Nature is full of remarkable nanoscale protein machines that can walk, talk, bind and self-assemble. As synthetic chemists, we have the opportunity to borrow from nature's vast catalogue of proteins, and modify their properties to create macromolecules that can perform completely new and useful functions.

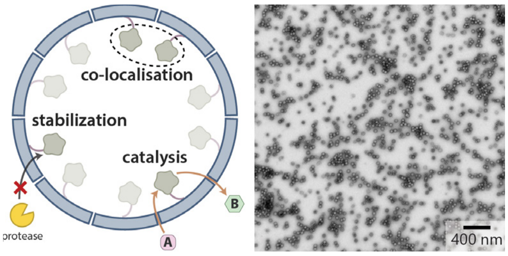
Encapsulin compartments as nanoreactors *(in collaboration with Dr Tobias Giessen from Harvard University and A/Prof Stephen Bell from the University of Adelaide):* Encapsulins are recently discovered bacterial proteins that spontaneously assemble into hollow 20-45 nm shells (see *Nat. Microbiol.* **2017**, 2, 17029). A unique feature of encapsulins is their ability to house other molecules, in a targeted binding process that is mediated by a simple peptide tag. We have been creating nano-sized reaction vessels by functionalising the interior of these shells with synthetic molecules that bear this peptide tag.

An example of our recent encapsulin work is featured in our publication on creating synthetic organelles inside living cells (*Nat. Commun.* **2018**, 9, 1131). We show that encapsulins can be used to stabilise and co-localise proteins within their interiors, and can also support enzymatic catalysis. We are now working on encapsulating biological catalysts of industrial relevance, such as p450 enzymes, and determining what effect the encapsulation process has on activity, chemical stability, and longevity of the enzymes.

Stapled peptide anti-cancer therapeutics: Stapled peptides are promising inhibitors of protein-protein interactions that are the drivers of many cancers. The stapling process involves the cyclisation of two unnatural amino acid side chains, imparting conformational rigidity which can improve proteolytic stability and cellular uptake. Our chemical approach to stapling involves using a double-click reaction, using a dialkynyl linker to bridge two azido amino acids.

Recent targets have included the tankyrase substrate recognition domain (*J. Am. Chem. Soc.* **2017**, 139, 2245-2256) and the Ctf4 hub of eukaryotic replication (*Angew. Chem. Int. Ed.* **2017**, 56, 12866-12872). Ongoing work in the group includes the detailed investigation of the cellular uptake and localisation of peptides into mammalian cells, and exploring alternative biosynthetic strategies to generate high-throughput libraries of stapled peptides.

The Bio-Incubator Hub: In collaboration with the group of Dr Shelley Wickham, we have established a shared hub for biomolecular research within the School of Chemistry. Technical capabilities we have established include lab-scale bacterial culture, DNA manipulation and analysis, and protein production and purification. This facility is available for all in the School to use, and should reduce the barriers to interdisciplinary research activities in the bio-nano research space.



Left: Encapsulin nanocompartments can be used to assemble nanoreactors with unique properties. Right: Transmission electron microscopy image of highly-monodisperse encapsulin compartments.

The groups of Dr Yu Heng Lau and Dr Shelley Wickham, who jointly run the new Bio-Incubator hub in the School of Chemistry.

PROFESSOR PETER LAY, FAA

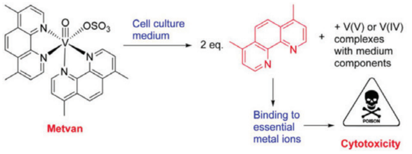
Our research is focused on biomedicine: understanding the mode of action of anticancer and anti-diabetes drugs; biospectroscopic studies on disease processes (including extracellular vesicles); disease diagnostics; and in vitro drug efficacy.

BIOINORGANIC CHEMISTRY

Anti-diabetic effects of chromium and vanadium *(Carter, Crans,* Kaur, Lai,* Lee, Levina, Mak, Safitri, Swarbrick, Tobin,* Vogt,* Young):* Speciation of Cr and V antidiabetic complexes in biological fluids, cells, and tissues has continued. Vibrational spectroscopic microbe techniques and capillary immunoassays (BLItz) 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 their anti-diabetic activities. 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 BLItztechnique 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, Ru and V anti-cancer drugs *(Andreichenko, Andrews,* Bader,* Carter, Chen,* Chetcuti, de Jonge,* Kalnina, Kuramarohit, Levina, Liang, Mak, Paterson,* Pei, Pham, Plush,* Rathje, Stewart, Swarbrick, Vogt,* Wood, Yaourtis, Zhang):* Research was conducted on Ga, Rh, Ru and V anti-cancer drugs using similar methodologies as those described for anti-diabetic drugs 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. Excitingly, some such drugs have exhibited irreversible differentiation of metastatic cells to non-agressive phenotypes. The speciation of different Ga prodrugs in blood, gastric juices and cells was examined using X-ray absorption spectroscopy. The BLItz technique to examine modifications of Tf/Tfr interactions, which showed that Tf is unlikely to mediate the uptake of these anti-cancer metal ions.

Molecular assays in disease diagnosis, pathogenesis and physiology in cells and tissues *(Al-Juaifari, Arora,* Austin,* Bader,* Carter, Chen,* Duong, Grau*, Hosseini-Beheshti, Hunt,* Lai,* Lee, Levina, Lin, New, Pamphlett,* Paterson,* Plush,* Vogt,* Zou):* Vibrational spectroscopic diagnostics for various diseases and conditions: including cerebral malaria; bacterial and viral meningitis and multiple sclerosis 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 imaging was used with synchrotron X-ray micro-probe techniques, to understand the disease biochemistry of some of multiple sclerosis and the role of microvesicles derived from monocytes on a variety of diseases.Methods have been developed for using Raman spectroscopy to obtain the history of medical and psychological effects from datelines in deciduous teeth.



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.

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.

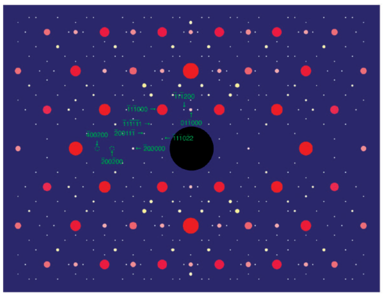
The goal of our research is to discover, characterise and optimise functional solid-state materials. Structure plays a central role, and we make particularly heavy use of neutron, synchrotron X-ray and electron diffraction as well as complementary techniques such as spectroscopy and electron microscopy.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

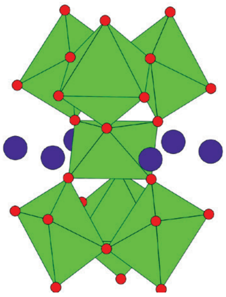
Solid-state ionic conduction in large single crystals

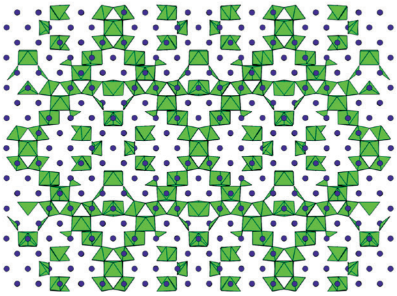
The high-temperature cubic form of bismuth oxide, δ-Bi_2O_3, is the best intermediate-temperature oxide-ionic conductor known. The most elegant way of stabilizing δ-Bi_2O_3 to room temperature, while preserving a large part of its conductivity, is by doping with higher-valent transition metals to create 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 NbO_6 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-Bi_2O_3-like channels, explaining the high oxide-ionic conductivity compared to commensurately modulated phases in the same pseudo-binary system.

Giant magnetoelastic effect in 5*d* 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.,* ZrW_2O_8), 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 $Ba_3BiIr_2O_9$ is an entirely novel case of the latter, magnetoelastic, case. Its structure contains face-sharing Ir_2O_9 bi-octahedra with direct bonds between Ir^{4+} 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 5*d* 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).







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: The over-arching theme in this area is the transformation of "waste" biomass into high specification fuels and platform chemicals. In conjunction with Professor Rocky de Nys (James Cook University) and Professor Moti Herskowitz (Ben Gurion University) we have shown that green macroalgae can be grown to remediate waste water and then converted to a drop-in diesel or jet fuel blend. In conjunction with Licella Pty Ltd (www.licella.com), which we co-founded, we have developed novel catalytic hydrothermal processes to upgrade of waste pine wood to, among other things, phenolic rich biocrude: capable of use in renewable resins and adhesives. Additionally, our collaborative work with Ca' Foscari University (Venice) has resulted in new molybdenum-based catalysts for the conversion of pulp and paper waste (Kraft lignin) to renewable aromatic chemicals: the starting point for many important chemical products.

With Professor Avelino Corma from the University of Valencia's ITQ we have shown how biocrudes can be successfully upgraded in conventional refineries with conventional catalysts.

New 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 – and a spin-out from our laboratory (Gelion Technologies Pty Ltd, www.gelion.com) seeks to commercialise this chemistry with a non-flow approach. We are using ionic liquid gels to access a range of attractive battery chemistries - pursuing both academic and commercial research.

Indeed, tailoring the properties of nanostructured Ionic liquid gels is our key approach for the design of novel battery systems. Furthermore, we are working towards the integration of improved battery storage systems with the built environment. Imagine your house, car and office with batteries inherently included as part of their structure, ready to take advantage of rapidly improving, solar energy technology and to serve as a buffer for the grid, enabling an ever-greater share of renewables to be connected, while grid stability is maintained.

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 engineer the band-gap of self-assembled nanostructures to provide better catalysts for this reaction. Our focus lies on two types of material. Graphitic carbon nitride has special semi-conductor properties and can be used for a variety of catalytic reactions including carbon dioxide activation as artificial photosynthesis and water splitting. We have now begun to use X-ray spectroscopy to characterize doped carbon nitride which have provided enhanced activity for these reactions, including X-ray photoelectron spectroscopy and X-ray absorption fine structure spectroscopy. Dispersed, TiO_2-stabilised exotic multicomponent nanoparticles and coupling these to reducing 'sacrificial' solutions that enhance the thermodynamics of the system. Such solutions can be readily found in the environment where they often present problems. Our approach yields hydrogen from water using sunlight and as a 'spin-off' improves the water quality by oxidising smelly and toxic species such as sulfides.

ASSOCIATE PROFESSOR TONY MASTERS

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

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 process, such as hydrocarbon oxidations. In applied studies, we collaborate with local industry to develop an Australian manufacturing capability for novel "ionic liquid" solvents. Representative projects are described below.

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

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, $H+ + e- \leftrightarrow ½H_2$) 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.

Mechanistic understanding of homogeneous catalysis: Understanding key reactions involved in homogeneous catalysis is hugely important to maximise their potential. In order to gain this information, it is important to probe reaction steps in situ and develop experimental methods to understand the nature of a catalyst in its real environment. This information will help develop much more stable and efficient catalysts, also look toward using more abundant elements such as nickel and iron, in replacement of much rarer metals. Recently we have used a variety of in situ methods to discover key underlying principles of an important nickel homogeneous catalysts for alkene isomerisation. This has given us a unique insight into its mode of action, helping move towards the replacement of platinum and palladium catalysts for cheaper, more abundant nickel-based compounds.

Photochemical conversion of CO_2 (with Prof Smith UNSW): We will prepare improved catalysts for the photochemical conversion of CO_2 to chemicals and fuels, using only sunlight and earth abundant materials to power and catalyse the reaction. This target reaction will lead to useable chemicals and promote a circular economy (e.g., promoting HCO_2H formation as a hydrogen carrier as we have described previously. We will achieve this aim through a combination of computational-chemistry-led catalyst design and Fermi energy control, advanced reactor design and materials synthesis, as well as the fine-tuning of the reaction media to increase the reaction rate.

ASSOCIATE PROFESSOR CHRISTOPHER MCERLEAN

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

SYNTHETIC ORGANIC CHEMISTRY

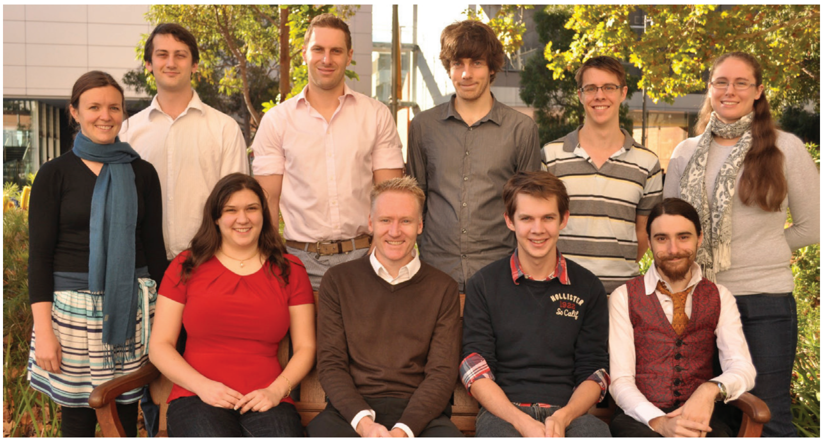
On-water chemistry *(Phippen, Norcott, Beare, Graham)*: Water is the most abundant liquid on our planet – we are surrounded by it. Yet when it comes to reactions, chemists traditionally use toxic, flammable and expensive fossil-fuel based solvents. We are working to change that. Environmental and safety 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 McErlean group



DR MARKUS MUELLNER

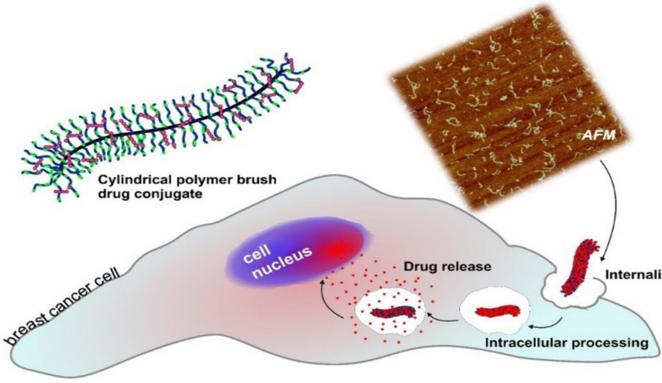
Our research uses controlled polymerisation techniques to construct polymer architectures and polymer assemblies to address key questions in a range of priority areas. A focus of our research is centred around molecular brushes and shape-anisotropic nanomaterials which is feeding into three key research interests: self-assembly, cellular interactions and hybrid materials.

FUNCTIONAL POLYMER NANOPARTICLES

Molecular polymer brushes in nanomedicine. The shape-persistent nature and cylindrical conformation of molecular polymer brushes (MPBs) present opportunities to explore the properties of anisotropic (i.e. non-spherical) nanomaterials in biological settings (Müllner et *al. Macromol Chem Phys* **2016**, *207*, 2209-2222 and *Polymer* **2016**, *98*, 389-401). MPBs allow their shape and rigidity to be altered, which in turn can be used to influence the *in vivo* circulation behaviour of brush polymer particles. Increasing the aspect ratio or altering the rigidity led to reduced exposure, higher clearance rates, and increased mononuclear phagocytic system organ deposition (Müllner *et al. ACS Nano* **2015**, *9*, 1294-1304). MPBs with lengths of up to 1 μm can passively target tumour xenografts via the enhanced permeation and retention (EPR) effect and extravasate into tumour tissue. Large CPBs with higher aspect ratios accumulated in tumours, with similar efficiencies to much smaller, spherical systems (Müllner *et al. Chem Comm* **2016**, *52*, 9121-9124 in collaboration with the Monash Institute of Pharmaceutical Sciences). The modular synthesis of MPBs further offers ample avenues to synthesise rod-shaped polymer particles for pH-responsive doxorubicin delivery to breast cancer cells (Pelras *et al. Polymer* **2017**, *112*, 244-251). Current studies focus on enhancing the tissue penetration of such drug delivery carriers, looking at particle charge, stiffness, and hydrophobicity.

Proapoptotic peptide nanoparticles. In collaborative work with the Nanostructured Interfaces and Materials Science group at the University of Melbourne, we developed a method to produce nanoparticles directly from functional peptides. Our versatile and robust approach produces proapoptotic peptide nanoparticles from mitochondria-disrupting KLAK peptides yielding highly functional therapeutics. The nanoparticles were designed to disassemble into free native peptides via the traceless cleavage of disulfide-based cross-linkers. The cytotoxicity of the nanoparticles can be tuned by controlling the kinetics of disulfide bond cleavage, and the rate of regeneration of the native peptide from the precursor species. Small molecule drug can be loaded into the nanoparticles to confer synergistic cytotoxic activity, further highlighting the potential application of KLAK particles in therapeutic delivery (Suma *et al. J. Am. Chem. Soc.* **2017**, *139*, 4009-4018).

Polymer Nanostructures Group 2017



Structured semiconductors for battery electrodes. Many properties of functional materials depend critically on their effective surface areas. We used a newly developed polymer-hybrid method to fabricate porous structured titania nanomaterials with high surface areas and efficient internal topologies. Our materials have shown performance enhancement as electrode materials in solid-state batteries – outperforming electrodes built from commercial titania components (in collaboration with Professor Chris Ling).

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.

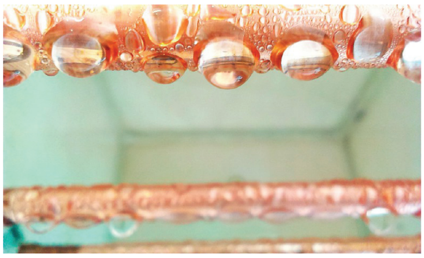
NANO INTERFACES

New polymer patterns for atmospheric water capture *(Al-Khayat, Chou):* We have established the optimal size and density distribution of polymer surface patterns for the collection of water from humid air. Dense, nanoscale hydrophilic bumps are not as efficient as more sparse micrometric bumps at collecting water. On the micrometric patterns the ideal conditions for water capture can be achieved with no energy input. We have applied our patterns onto three-dimensional substrates (shown copper tubes) and quantified water collection under realistic atmospheric conditions.

Self-assembled monolayers on different solid substrates *(Hong, Nelson, Wood):* We have developed an in-peth understanding of self-assembled monolayer films that form on solid surfaces using halogen bond interactions. The strong adsorption of perfluorinated alkanes produces hydrophobic surfaces with extremely low free energy, which might be able to provide useful electronic properties when added to semiconductor surfaces. 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.

Fouling and drag reduction by slippery liquid infused surfaces *(Peppou-Chapman, Scarratt, Smith-Palmer, Owais):* Slippery liquid infused surfaces formed through the spontaneous wrinkling of a rigid Teflon film (which mimic the surface of the pitcher plant as shown in figure 2) were fabricated and their functional properties investigated. The produced wrinkled surfaces were shown to dramatically inhibit the attachment of marine fouling bacteria, prevent fouling by oils, and have promise to significantly reduce interfacial drag of liquids. Their robustness compares well with commerical coatings used currently for different advanced applications.

Polymeric Janus nanoparticles *(Hawkett, Zhu, Nguyen):* The synthesis of polymeric Janus nanoparticles has been refined to the point where we can now produce new materials that are beneficial to the paint industry. In our ARC Linkage grant with Dulux Australia we have shown that they offer multiple and advanced functions.



Copper tubes

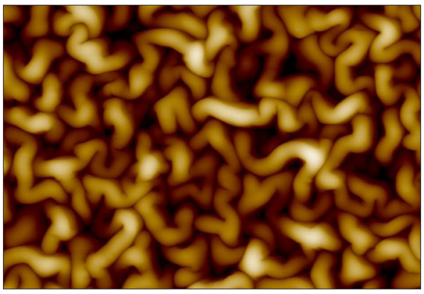
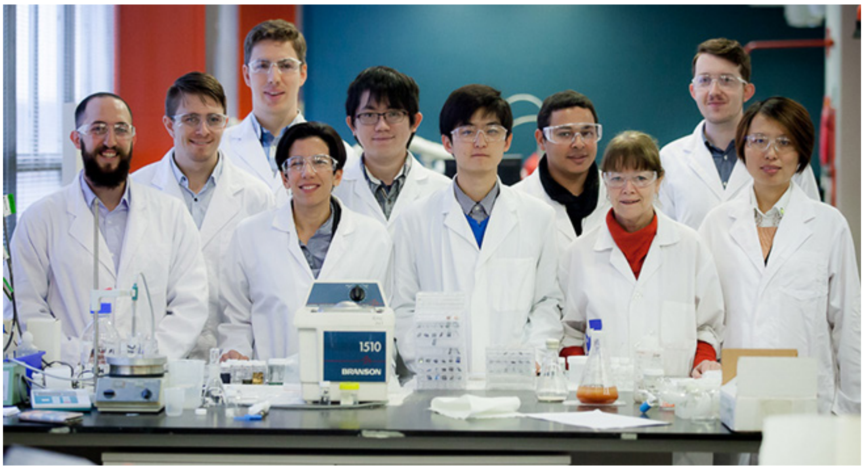


Figure 2

The Neto group 2017



ASSOCIATE PROFESSOR ELIZABETH NEW

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

Fluorescent sensors based on 1,8-naphthalimides *(Chrzanowski†, Jolliffe, Leslie, Shen, Yang):* 1,8-Naphthalimides are green-emitting fluorophores commonly used in responsive sensors, including in our redox-responsive probes. We have reported modified structures with greatly expanded photophysical properties (*Chem. – Eur. J.*, 2018, 24, 5569), and have used these properties to design hypoxia sensors (*Org. Biomol. Chem.*, 2018, 16, 619).

New fluorescent sensors for the study of oxidative stress in biology *(Fraser†, Ghrayche, Lay, Lin, Trinh):* We have continued in our quest to understand how perturbations in cellular redox state are related to disease, focussing primarily on how we can target our probes to specific sub-cellular organelles. We have also extended our network of collaborators who are applying our probes in various biological studies including stem cell differentiation, bacterial infection, neurodegeneration and cancer.

Responsive magnetic resonance sensors *(Bonnitcha, Harris, Kolanowski, O'Neill):* Magnetic resonance imaging (MRI) offers the possibility of high resolution, whole animal imaging. We are developing gadolinium-based MRI contrast agents that respond to hypoxia and oxidative stress. We are also investigating novel cobalt systems, including hypoxia-responsive (*Inorg. Chem, 2017,* 56, 9860) and anion-sensitive systems (*Chem. Commun.*, 2017, 53, 3571).

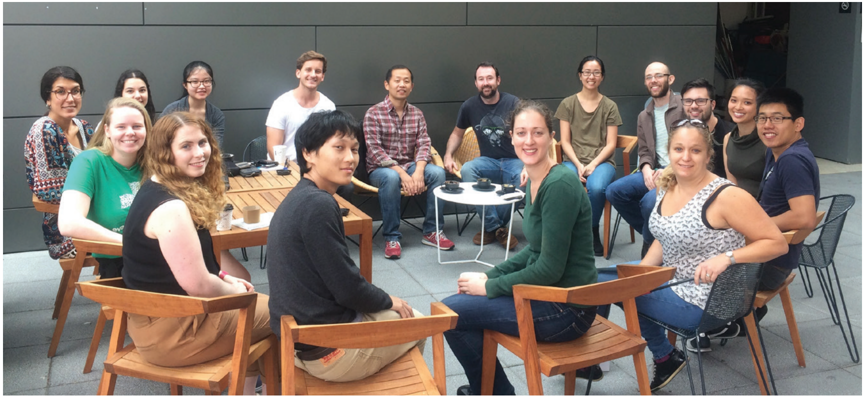
The effects of cancer treatments on labile metal pools *(Akerfeldt, Carney, Chan, Graziotto, Hambley Kolanowski, Shen):* We are developing probes for biologically-relevant metal ions, that can be used to provide information about how labile metal pools change with chemotherapy. For example, we have developed and used a ratiometric iron sensor to study the efficacy of iron chelation therapy (*Metallomics*, 2018, DOI: 10.1039/C7MT00297A) and have uncovered changes in subcellular copper distribution in response to cisplatin treatment (*J. Biol. Inorg. Chem.*, 2017, 22, 765).

New methods to study platinum anticancer therapy *(Graziotto, Hambley, Kolanowski, Lim, Mitchell, Roberts†, Wang):* 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 (*Sens. Actuators, B*, 2018, 255, 2721). We have also applied size exclusion chromatography inductively-coupled plasma mass spectrometry (SEC-ICP-MS) to investigate interactions of platinum complexes with cellular proteins (*J. Inorg. Biochem.*, 2017, 177, 328).

Fluorescent sensing arrays *(Jolliffe, Mitchell, Smith, Zwicker):* Cross-reactive arrays of fluorophore enable the sensing of complex fluids that contain many similar analytes (*Analyst*, 2017, 142, 3549). We are working on a range of methods to generate diversity of sensing elements to measure analytes in environmental and biological samples.

† collaborators from outside the School of Chemistry

The New group, 2017



PROFESSOR RICHARD PAYNE

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

ORGANIC SYNTHESIS, DRUG DISCOVERY & CHEMICAL BIOLOGY

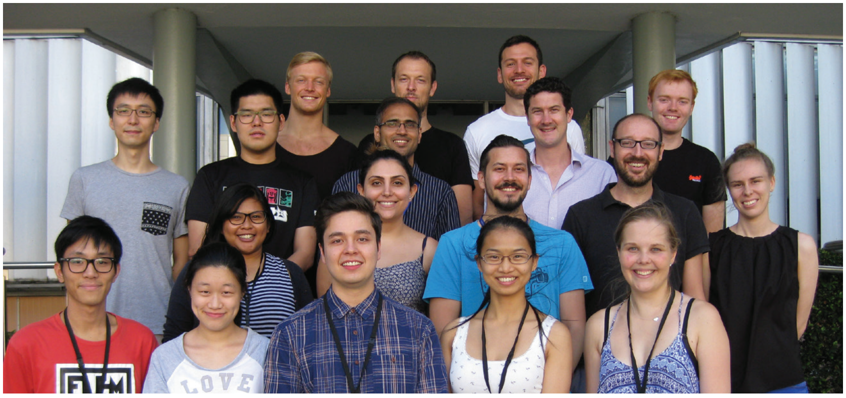
Tuberculosis drug discovery *(Dowman, Elias, Giltrap, Hawkins, Tran, Watson, Britton): Mycobacterium tuberculosis*, the etiological agent of tuberculosis (TB), is a devastating human pathogen. Every second a new person is infected with *M. tuberculosis*, resulting in close to 2 million deaths from TB 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, Premdjee, 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 anti-thrombotic 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.

Payne Research Group



PROFESSOR LOUIS RENDINA

Our research group is primarily interested in synthesis and the medicinal chemistry of boron and the lanthanoid elements, particularly gadolinium.

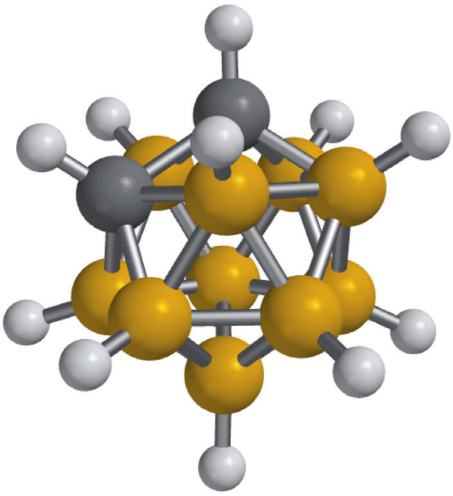
SYNTHESIS AND INORGANIC DRUG DISCOVERY

Our research group has a strong interest in synthesis and the design 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 *(Hall, Harris†, Robertson):* An important breakthrough made by our group opens up new horizons in the delivery of Gd to tumour-cell mitochondria for potential application as new 'theranostic' agents for PAT, NCT and MRI. 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 for T98G cells over normal, human glial (SVG p12) cells. Significant numbers (> 10^{10}) of Gd atoms (equating to ca. 3 x 10^{3} ppm) can also be delivered to a single T98G cell. Importantly, *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 *(Dasgupta, Kassiou, Kavianpour):* 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) and histone deacetylase (HDAC) enzymes which are directly involved in tumour immunity escape and tumour cell epigenetics, respectively.

New boron fluorophores for near-IR biological applications *(Marfavi, New):* 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.



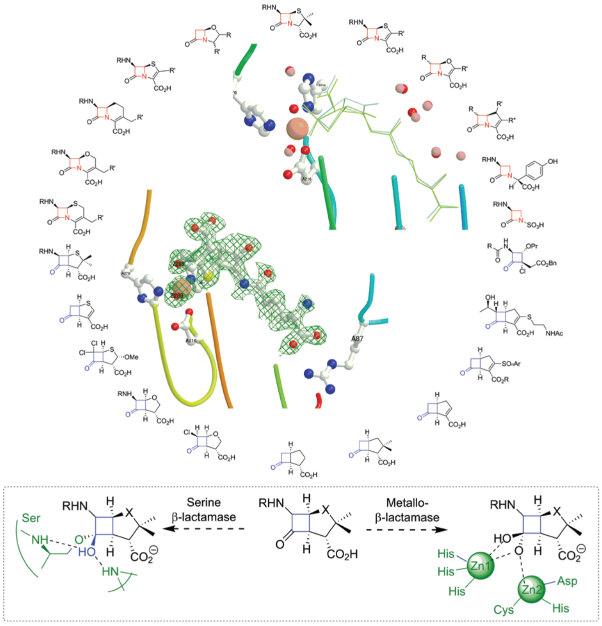
ASSOCIATE PROFESSOR PETER RUTLEDGE

Our research combines organic synthesis and bio-organic chemistry to develop new drugs and sensors for biomedical applications, chemical solutions to environmental problems, and biologically-inspired catalysts for synthesis.

MOLECULAR PROBES & SENSORS

In 2017 we reported an effective method for monitoring ligand displacement in cyclam-scorpionand complexes using NMR, an important step forward in our search for chemical probes to visualise interactions between small molecule ligands and biomolecules (*Eur. J. Inorg. Chem.* **2017** 1075, 2017, with Joseph Wong, Nicholas Proschogo and Mat Todd). Our approach exploits anion-induced ligand displacement to trigger coordination changes, and ^{1}H and ^{2}H NMR to follow these changes. Extending this idea further, we have just reported a series of 'molecular switches for any pH' that utilise the versatile coordination behaviour of cyclam-scorpionands and ligand displacement via changes in protonation state (*Chem. Eur. J.* **24** 1573, 2018, with Yu Heng Lau, Jack Clegg, Jason Price, Rene Macquart and Mat Todd).

Our work on smartphone sensing with John Canning (interdisciplinary Photonics Laboratories, iPL) and Abbas Jamalipour (School of Electrical and Information Engineering) continued in 2017, to include time-resolved and temperature tuneable measurements on a smartphone fluorimeter (*Analyst* **142** 1953, 2017, with Arafat Hossain, Zhikang Yu, Sandra Ast and Joseph Wong).



Cyclobutanone Analogues of β-Lactam Antibiotics: β–Lactamase Inhibitors with Untapped Potential? P. Devi & P. J. Rutledge ChemBioChem ***18*** *338 (2017). DOI: 10.1002/cbic.201600529*

ANTIBIOTICS

We completed a comprehensive review of cyclobutanone analogues of β-lactams, and their capacity to inhibit β-lactamase enzymes and thus combat the burgeoning threat of antimicrobial resistance (*ChemBioChem* **18** 338-351, 2017, with Prarthana Devi and Nicole Groves). Our article brings together >35 years of research on cyclobutanones, which are isosteric with β-lactams - the eponymous cyclic amide of the lactam is replaced with an all-carbon ring - and have been explored as prospective antibiotics and as inhibitors of β-lactamases and other serine proteases (Figure 1).

Work also continued to investigate structure/ activity relationships in our cyclam-derived antitubercular agents (*J. Med. Chem.* **59** 5917, 2016) and demonstrate efficacy in *in vivo* models (with Malcolm Spain, Joseph Wong, Jamie Batten, Gaya Nagalingam, Xiao Fan Jiang, Hasini Murage, Jack Orford, Patrick Crisologo, Mat Todd and Jamie Triccas).

In natural products discovery, in 2017 we isolated and characterised more than a dozen new and not-so-new secondary metabolites with a range of interesting structures and biological activity from terrestrial and marine organisms (with Mojdeh Dinarvand, Diana Quan, Jamie Triccas; Heather Lacey, Rob Baker, Ian Luck, Nick Proschogo, David Antonjuk and Ern Lacey, Microbial Screening Technologies, MST).

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.

INORGANIC SOLID STATE CHEMISTRY AND CHEMISTRY EDUCATION RESEARCH

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 in such rechargeable battery systems 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 lead-free 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. Composition and temperature dependent phase transitions were determined in all systems. Ferroelectric properties were investigated for selected samples.

Nanostructural investigation of dental-filling materials *(Loy, Matori†, Zainuddin†):* Glass ionomer cement (GIC) is the standard dental filling material. The aim of this project is to investigate the polymer-glass-hydrogel phase evolution of freshly-made GIC pastes by using Ultra Small Angle Neutron Scattering in conjunction with Small Angle Neutron Scattering, FTIR and Field Emission SEM. GIC paste has a complex structure, which consists of polyacrylate, glass, hydrogel and air phases. The phase evolution of GIC pastes affects the pore structure and mechanical properties of GIC. The combination of techniques is necessary to study the cement phase evolution and pore structure of GIC pastes in the expected length scale of 2-400 nm. The nanoscale features of GIC pastes are important to interpret our closely related results from nanoindentation and compressive strengths tests. The thermally induced amorphous-to-crystalline transition of fluoroaluminosilicate glass to fluorapatite glass-ceramic is also investigated to determine the morphology of the fluorapatite phase in the glassy matrix.

† *Collaborators from outside the School of Chemistry*

1. T. A. Whittle, W. R. Brant, J. R. Hester, Q. Gu. & S. Schmid, *Dalton Trans.* (2017). Tailoring phase transition temperatures in perovskites via A-site vacancy generation. DOI: 10.1039/c7dt00352h
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3. D. T. Murphy, S. Schmid, J. R. Hester, P. E. R. Blanchard & W. Miiller, *Inorg. Chem.* (2015). Co-ordination site disorder in spinel-type $LiMnTiO_4$. DOI: 10.1021/ic502747p

ASSOCIATE PROFESSOR MATTHEW TODD

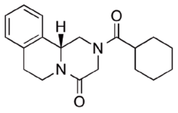
We discover new ways to make molecules, either by studying reaction mechanisms or designing catalysts. Many of the molecules have uses as treatments for tropical diseases or as sensors for deployment in cells. We are devising new, open ways to carry out this research that allows anyone in the world to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

ORGANIC SYNTHESIS, CATALYSIS AND MEDICINAL CHEMISTRY

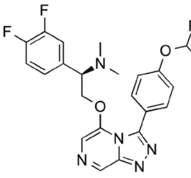
The Open Source Malaria Consortium: We recently demonstrated an important proof of concept – that a challenging research problem can be solved more quickly if the research is carried out openly and anyone can contribute. The problem was the preparation of an important drug for the neglected tropical 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.[1] Despite there being no patents on our discovery it is being developed by a company for the international market and has furthered research in the private sector.

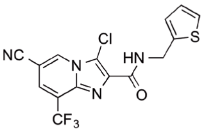
We have extended this idea to *open source drug discovery*. With the Medicines for Malaria Venture, GlaxoSmithKline and a wide range of people who have spontaneously joined the project, we have prosecuted hit-to-lead campaigns in antimalarial drug discovery where all data and ideas are freely shared: The Open Source Malaria (OSM) Consortium.[2a] We have devised a technical platform applicable to any transparent, patent-free research endeavour.[2bc] The consortium recently published its first major research paper describing a new series of potent antimalarials,[2d] and is now working on a different series with *in vivo* efficacy. This prize-winning[2e] research demonstrates a new way to discover medicines that we have begun to apply to other diseases such as tuberculosis.[2f] More broadly we have proposed a roadmap towards Open Source Pharma[2g] as a competing model for the traditional pharmaceutical industry, and were awarded $4M from Tata Trusts to establish a foundation in India to support open source projects around the world.[2h] In 2016 Dr Alice Williamson and I, with the rest of the OSM community, worked with students from Sydney Grammar School to enable them to complete the synthesis of an expensive drug, an achievement that was widely reported in the media.[2i]



Schistosomiasis
(*R*)–Praziquantel



Open Source Malaria
MMV670437, 44 nM



Open Source TB
TCMDC143693

Responsive metal complexes: My group pioneered a new kind of coordination compound that changes its shape in a defined way when it binds a biological molecule.[3] 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,[4a-c] in particular following up a serendipitous discovery of their potency vs. drug-resistant tuberculosis.[4d]

References:

1. a) *Nature Chemistry* **2011**, *3*, 745; b) *PLoS Negl. Trop. Dis.* **2011**, 5(9): e1260

2. a) opensourcemalaria.org; b) *Parasitology* **2014**, *141*, 148; c) *Chem. Sci.* **2015**, *6*, 1614; d) *ACS Central Science* **2016**, *2*, 687; e) http://youtu.be/gCOokjOiVTc; f) *PLoS ONE* **2014**, 9(12): e111782; g) *PLoS Med.* **2017**, *14*(4): e1002276; h) http://tinyurl.com/n7zkhrf; i) http://tinyurl.com/daraprim

3. *Chem. Eur. J.* **2009**, *15*, 3720

4. a) *ChemBioChem* **2013**, *14*, 224; b) *Eur. J. Inorg. Chem.* **2012**, 5611; c) *ChemistryOpen* **2013** *2*, 99; c) *Metallomics* **2014**, *6*, 1931; d) *J. Med. Chem.* **2016**, *59*, 5917.

PROFESSOR GREGORY WARR

We investigate how macroscopic properties and functionality arise by interrogating the nanoscale structure of soft matter using neutron and X-ray beam techniques.

IONIC LIQUIDS AND LOW WATER-ACTIVITY SOLVENTS

(Jiang, Bryant, FitzGerald, Atkin, Chen,* MacDonald,* Imberti,*):* In our work we explore unconventional liquids and solvents typified by room-temperature ionic liquids (ILs) – salts that melt near or preferably below room temperature. We focus on understanding how their unique physical and chemical characteristics arise from their nanoscale structure, and how that can be designed by manipulating molecular structure and intermolecular forces.

Using neutron diffraction at the Rutherford Appleton Laboratory in the UK alongside molecular simulations, small-angle neutron scattering at the ANSTO Opal reactor, and X-ray scattering in our own laboratory, we have found striking changes can be introduced into IL structure by changing organic cation or anion or by mixing salts or organic molecules. These impact on the properties of ILs, and their use for a wide range of applications from synthesis and catalysis to bioprocessing and energy storage. Recently we have shown that surface structure can induce the spontaneous exfoliation of layered materials into 2D nanomaterials such as graphene.

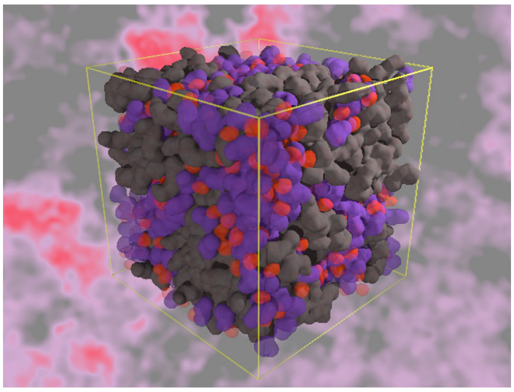
A key property of ILs and their solutions is that their liquid phase is stable over a wide temperature range, and that they have remarkably low vapour pressures, so do not evaporate. This often comes at the cost of incorporating environmentally-unfriendly components, such as fluorine-rich anions. Our work focusses on a more sustainable approach incorporating bio-friendly materials such as ILs built from simple organic salts, including choline, carboxylic and amino acids, and incorporating low-volatility molecular components such as urea, glycerol or water bound into the liquid by strong intermolecular forces. These include both solutions and deep eutectic Solvents (DES). DES are mixtures of two high melting-point components, usually, a salt and a molecular H-bond donor that form a stable liquid far below the melting point of either pure component.

Our work has shown how the liquid structure of ILs and related mixtures differ from simple electrolytes, frequently containing clusters of polar and non-polar groups arranged into extended nanoscale domains. A key outcome has been to show how the presence of these two immiscible domains aids in the dissolution of complex solutes, with important implications for bioprocessing such as the extraction of lignins, and how to optimise the design of new IL-based solvents.

ILs and DESs are also remarkable in their ability to support the self-assembly of complex, amphiphilic solutes like surfactants, lipids and block-copolymers. Although many exotic solvents 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 that have no parallel in water, as well as supporting conventional amphiphilic self-assembly into micelles, vesicles and liquid crystals, heralding a new class of solvents for novel forms of soft matter.

As self-assembly is a form of compartmentalisation widely regarded as a necessary precursor to the origin of life, we have explored a range of extreme conditions to explore where life might either arise or be artificially suspended and sustained. We have investigated lipid bilayer formation, stability and the function of simple biomolecules function in ILs and DESs showing, for example, how selective ion transport can be preserved in these nonaqueous media.

Loading ionic liquid samples onto the small angle neutron diffractometer for amorphous and liquid samples (SANDALS) at the Rutherford Appleton Laboratories in the UK.



Simulation box describing neutron diffraction results showing the interpenetrating domains of polar groups (-OH; -NH3+; NO3- in red) and the non-polar propyl (purple) and octyl (grey) chains in mixtures of the IL propylammonium nitrate with n-octanol.

DR SHELLEY WICKHAM

Our group uses DNA as a molecular building block for self-assembling nanoscale structures and devices, for applications as tools for single molecule biophysics, platforms for diagnostics and therapeutics, and templates for nanofabrication.

DNA ORIGAMI

DNA origami is a method for making 3-dimensional DNA nanostructures with arbitrary shapes by folding up a long single-stranded DNA ‘scaffold’. Custom DNA origami nanostructures can be designed as tools for specific biophysical measurements. For example, a DNA origami nano-spring, which was used to simultaneously measure force and position of the protein motor Myosin VI during stepping (Nat. Commun. **2016**, *7*, 13715).

Our current research focuses on hierarchical assembly of many DNA origami components into much larger assemblies. These nanostructures can act as versatile nanoscale pegboards for applications requiring complex 3D arrangements of matter, with as many as 2000 uniquely addressable pixels spaced 9 nm apart. For example, they have been used to template polymer nanowires as components for nano-electronic circuits, and decorated with proteins to study the shape-dependence of nanoparticle interactions with cells.

DNA NANOTECHNOLOGY TOOLS

DNA nanobots for drug delivery *(in collaboration with A/Prof Ali Abbas, USyd Chemical Engineering):* We have designed a DNA origami nanobot, which is a multifunctional construct with the ability to carry payloads (eg. siRNA, endosomal escape agent), target specific cancer cells, and respond to external stimuli (eg. radio frequency (RF)). It can be modified to carry many different cargos, or to respond to different cell surface signals, depending on the target type. Our group is currently working on the controlled melting of gold nanoparticle–DNA complexes using RF, and in vitro targeting to specific cancer cell lines using DNA aptamers.

Top-down meets bottom-up *(in collaboration with Prof. Marcela Bilek, USyd Physics, and Dr. Anna Waterhouse, Heart Research Institute):* We are working to combine the strengths of top-down and bottom-up nanofabrication to build hybrid structures. In traditional top-down nanofabrication, large systems pattern a semiconductor substrate to build up sophisticated devices. In contrast, in the emerging field of bottom-up nanotechnology, clever design of molecular interactions drives the self-assembly of smaller building blocks into more complex structures, with smaller features. We are bridging the gap between these two technologies by assembling DNA origami nanostructures onto lithographically patterned substrates to build integrated devices. These devices will be applied, for example, to understand biological problems such as why blood clots form on implanted medical devices - their main cause of failure.

BIOMOD

(in collaboration with Dr Alice Williamson, USyd Chemistry, and Dr Anna Waterhouse, Heart Research Institute): BIOMOD is an annual international biomolecular design competition held at UCSF in San Francisco, CA, where teams of undergraduates build innovative and functional nanoscale devices using the molecules of life. Previous projects have used DNA, RNA, and proteins as building blocks to create nanoscale robots, molecular computers, and nano-therapeutics. Our group in the School of Chemistry is home of the USyd BIOMOD team. In 2017 a team of 6 students from Engineering, Arts and Science worked together to build a rapid point of care diagnostic device, and received a Gold Project Award in recognition of the quality of their scientific results and presentation, which placed them in the top 7 of teams internationally.

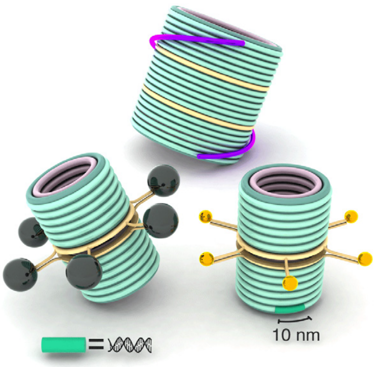


Figure 1: DNA origami barrels assembled with gold or iron oxide nanoparticles

The Sydney DNA group. (L-R) Shelley Wickham, Minh Tri Luu, Michael Rinaudo, Jasleen Daljit Singh

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.

THEORETICAL AND COMPUTATIONAL NANOSCIENCE

Ligand-mediated interactions between nanoparticles *(Hagan, Smith, Jiang, Monego, Geissler – U.C. Berkeley, Mulvaney – U. of Melbourne, Kraus – INM Saarbrücken):* 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.

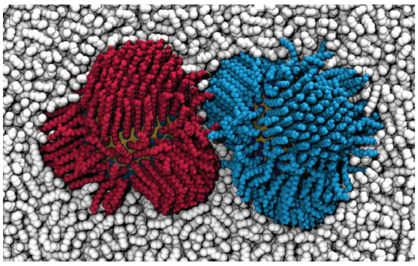


Figure 1. The aggregation of small Au nanoparticles in decane is driven by attraction between ligand monolayers on their surface.

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. We are now working with experimental collaborators in Australia and Germany to characterise this behaviour in dispersions of Au and CdSe particles (Fig. 1), and have so far been able to use our molecular-scale insight to explain a range of unexpected results. This includes a transition from ligand- to core-dominated aggregation as the particle size increases, which leads to an inversion of the effect of ligand length on particle stability, and solvent dependencies that run counter to the predictions of conventional colloid theory.

Our results add to a growing body of evidence that ligand-mediated interactions can exert a particularly strong influence on the solution stability and assembly of nanoparticles.

The group 2017

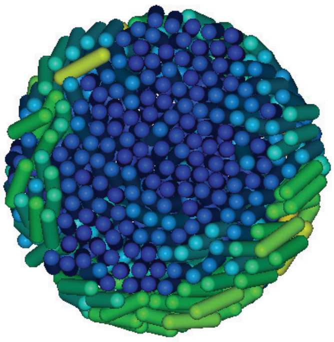


Figure 2. Rod-shaped nanoparticles can assemble into liquid-crystal-like aggregates in solution and at interfaces. We are investigating how this can be used to print materials with anisotropic transport properties.

Assembly of nanorods for solar energy applications *(Young, Wood, Modestino – New York University 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 collaboration with experimentalists in the United States who have used SAXS to study self-assembly in rod/polymer mixtures.

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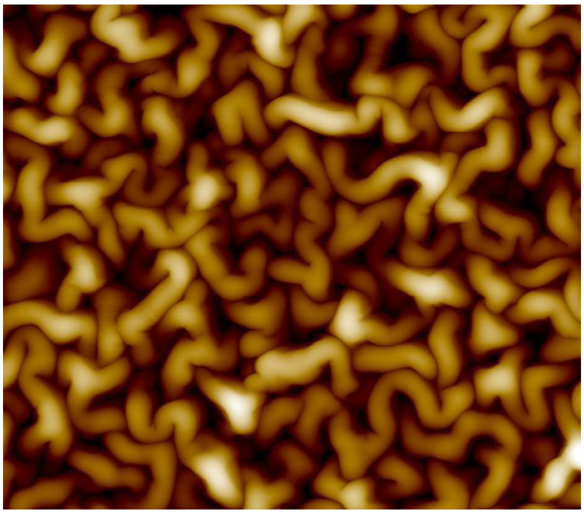

Courtesty of A/Prof Chiara Neto

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2017 Postgraduate Teaching Fellows

Jordan Darcy
Luke Dowman
Nabiha Elias
Cameron Hanna
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Pierre Naeyaert
Edward O'Neill
Julia Polt
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STUDENT PRIZES AND SCHOLARSHIPS

The School of Chemistry awards over $85 000 in Prizes and Scholarships each year to the best of its students. The following students were awarded prizes or scholarships for academic achievements at an awards ceremony held on 7 August 2017 based on their academic achievements in 2017 and 2018. Scholarships are awarded subject to the students satisfying conditions required for each of the individual scholarships.

Agnes Campbell Prize

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

Honours:

Timothy Callis
Timothy Chisholm
Claire Flitcroft
Joy Ghrayche
Jason Johansen-Leete
Jiarun Lin
Anita Marfavi
Genevieve Sergeant
Natalie Trinh

Postgraduates:

Neanne Alnafta
James Batten
Jonathan Chung
Luke Dowman
Charlotte Franck
Cameron Hanna
Paige Hawkins
Annukka Kallinen
Timothy Katte
Paul King
Kathryn Leslie
Rebecca Mattison
Linda Mitchell
Alexander Norman
Robert Rodger
Elisaabeth Tondl
Wendy Tran
Edwin Tse
Nikki Tzoumous
Xiaoyi Wang
Emma Watson
Anne Withecombe
Kylie Yang
Martina Yousif
Qingqing Zhou
Eddie (Vincent) Zwicker

Arthur Hollis Memorial Prize

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

Maggie Tong

Michael Liu

Australia-USA Foundation Prize

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

Catherine Doherty

Bruce Veness Chandler Research Support Scholarship in Food Chemistry

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

Claire Filtcroft
Joy Ghrayche
Marcus Graziotto
Paige Hawkins
Michael Moir
Philippe Nashar

C.H. Wilson Prize for First Class Honours in Organic Chemistry

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

Timothy Chisholm

Charles E. Fawsitt Prize for Chemistry

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

Daniel Cheung

Edna Maude Goulston Prize in Organic Chemistry

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

Timothy Chisholm

Frank E Dixon Scholarship in Chemistry

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

Stone Woo

George Harris Scholarship

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.

Alfonso Ballestas Barrientos

Maggie Corrigan

Theophile Pelras

G.S. Caird Scholarship in Chemistry

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.

Joshua Maxwell

Hush Prize in Theoretical Chemistry

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.

Alexander Hawken

Inglis Hudson Scholarship (Major) for Chemistry

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.

Stone Woo

Joshua Maxwell

Yi cheng Zeng

Inglis Hudson Scholarship for Chemistry

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.

Amy Bowyer

Sarah Bowyer

Lachlan Adamson

Iredale Prize

Awarded for outstanding merit in both a Semester 1 and a Semester 2 Core Intermediate Chemistry unit of study.

Maggie Tong

Michael Liu

Janet Elspeth Crawford Prize in Chemistry

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

Claire Wallace

Joan R Clark Research Scholarship

The Dr Joan R Clark Research Scholarships are supported by the income from gifts by Dr Joan R Clark, a distinguished mineral crystallographer who was formerly on the staff of the United States Geological Survey. The purpose of the Scholarship is to assist a postgraduate student proceeding to a Doctorate in the School of Chemistry to undertake research in connection with his/her doctoral thesis topic at a leading university overseas for a period of not less than six weeks.

Patrick Doheny

John A. Lamberton Research Scholarship

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

TBA

TBA

TBA

TBA

Levey Scholarship No. II (Major) for Chemistry

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

Shilan Ye

Levey Scholarship No. III for Chemistry

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

Zihao Qin

R.J.W. Le Fèvre Research Travelling Scholarship

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

TBA

TBA

TBA

Le Fèvre Student Lecture Awards for 2017

This lecture was established in 1985 following a gift of $2 000 from Emeritus Professor R.J.W. Le Fèvre and is awarded on the recommendation of the Sydney University Chemical Society.

Jessica Sayers

Marlowe Graham

Haihui Joy Jiang

Surface Coatings Association Australia Scholarship

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).

Sam Peppou Chapman

Walter Burfitt Scholarship No. 1 in Chemistry

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

Joshua Maxwell

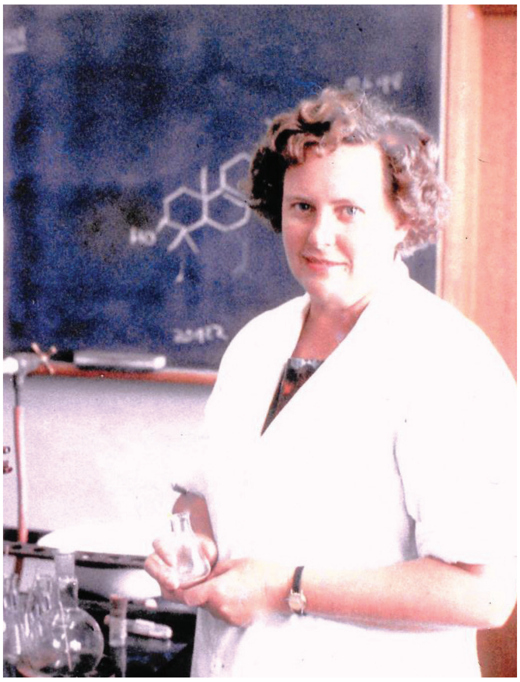
Walter Moore Honours Scholarship

Awarded on the basis of outstanding academic merit to a student enrolled in the School of Chemistry Honours Program.

Keiran Gerathy

Shurui Miao

Reginald Young



Ruth Gall nee Lack (1923-2017)

WE REMEMBER RUTH GALL (NEE LACK)

BY DR JOHN COLL (AM) DSC(1987) PHD(1969) BSC(1966)

Ruth Edna Lack was born in Pennant Hills, northwest Sydney on 8 November 1923. She passed away on 10 July 2017, at The Terraces, Varsity Lakes overlooking Bond University on the Gold Coast. She had lived a full and rewarding life of 93 years.

Ruth's father was a 'reluctant' Chartered Accountant, who Ruth believes would have been happier as an engineer or mechanic. He did not want her to become an Accountant. He involved his children in physics experiments and stirred their interest in many other things. He was an ardent tennis player, something Ruth emulated in later life. He loved a challenge. Her mother played the piano and the family and friends enjoyed singalongs around the piano, long before TV and karaoke. After losing about a year after a chance encounter with a Mark Foys' truck as a five year old, she completed her schooling to leaving certificate at Meriden School in Strathfield. She was always in the top two or three at school. Meriden School didn't offer the girls subjects like Physics and Chemistry.

On completion of her high school education during the first two years of the war, she initially took a job at Phillips Electrical Co at Edgecliff. During this time Japanese submarines were in Sydney Harbour, and she realised how real the war was. She decided to enlist in the Woman's Auxiliary Air Force (WAAF). She did basic training in Robertson and Bankstown, before being assigned to radar operations in Bowen, North Queensland, after a brief stay in Townsville to learn the ropes. She was on duty there until the end of 1944, when she was allowed to study Science at University of Sydney under the Commonwealth Reconstruction Training Scheme. Jan Morris, another former WAAF, joined her as students of Science with a lot to learn. Ruth struggled with Chemistry, managing a Pass at the end of the year, but was a Chemistry III and Chemistry III Advanced student by 1947. She attributed her transformation to the wonderful lectures given by Ern Ritchie and Frank Lions. An amazing achievement, considering she had no high school background in Chemistry. Obviously Chemistry had her in its thrall.

She spent two and a half years working in Sydney at CSR Chemicals and Union Carbide's predecessors in the Rhodes area, largely in quality control, after which, she decided to go to London where she worked at British Industrial Solvents. While the job was interesting, she eventually felt the need to return to Australia. She accepted a position at CSIRO's Coal Research Division, but found that this did not capture her imagination. Finally, she was encouraged by Sev Sternhell, then at Coal Research, to go back to University of Sydney as a Teaching Fellow while she pursued her Doctorate in Organic Chemistry. Prof Charles Shoppee, the world renowned Steroid Chemist who interviewed and appointed her, offered to supervise her studies.

She had reached her destination, after a long and unusual journey. Professor Shoppee mentored his colleague after her PhD studies were finished, and she in return supervised many of his students until his departure for Texas. Ruth completed her PhD in 1961 and became a Lecturer in Organic Chemistry in 1962, Senior Lecturer in 1966, and became Sydney University's first female Associate Professor in Chemistry in 1970.

After an Honours Year project under Ruth's supervision on attempts to convert lanosterol from wool wax into useful steroid precursors, Norm Hughes and I moved into 'The Professor's Laboratory', next to the office, which thereafter became known as the 'BullDog Lab', after 'Bull' Hughes and 'Mad Dog' Coll. Barry Newman and Frank Johnston had left, and the formerly peaceful lab was never quite the same. Music, visitors, etc seemed normal to us, but the Professor occasionally commented. Ruth was always dropping in, encouraging us to greater achievements and using natural competition between peers to great effect. Her time in the Airforce, and in Industry had not been wasted. She was a wonderful supervisor and constant source of ideas ('Thought of something in the shower this morning', 'Why don't we/you try this…'). It was an exciting experience working with 'Aunt Ruth', as she was affectionately known. Even on the social level, we might have a group dinner at her place, and it would become a contest to see who could make the best Pavlova against Ruth's previous efforts. We could all make Pavlova by the time we went on Postdoctoral travel overseas.

Organic Chemistry dinners were another memorable experience. Professor Shoppee always attended, and most thought he was pretty conservative. One time Len, Gary and other students were balancing wine glasses on top of each other to see how many they could balance. A waiter from the University Club came and chided them, so Professor Shoppee started balancing the glasses. He was left alone. He may have seemed a snob to some, but he was always loyal to 'His Staff', while still being 'The Professor'. I have learned a great deal from my supervisors, Professor Shoppee, and especially Dr Ruth Lack. I hope that made me a better supervisor to my students and staff over the years.

She was elected first female Head of School of Chemistry in in December 1978 by all Staff of the Chemistry Departments, and she served this role with distinction. She once told me that she was waiting to see the Vice Chancellor on a School matter. His Secretary wondered if she had an appointment, as Professor Gall had the next appointment that morning. She said:' I am she!"

She had received her DSc in Organic Chemistry in 1977, the first woman to be so honoured at the University of Sydney in this field. She was an inspiration to female students and staff, and although not a 'bra burning' feminist, she was a female trailblazer and role model for academic women.

She was the author of more than 70 publications and a wonderful supervisor and inspiration to many.

Ruth married Harold Gall, and became Professor Gall from this time. She was extremely happy until Harold's untimely passing in 1984, shortly after her retirement in 1982. Ruth stayed in Sydney for some time before beginning a slow migration northwards. Each year she would still drive her Honda back to visit friends in Sydney. She spent time in Coff's Harbour where a number of former students and friends visited, then Kirra, Robena Heights and finally Palm Beach. She was active in running courses on computer use over the years, enjoyed cards and the occasional foray into oil painting, and glazing ceramic objects which she had painted. She was a multi-talented person, who had long periods of physical discomfort, perhaps arising from the childhood accident. She moved from Palm Beach to her final residence at the Terraces.

Further reading: https://bit.ly/2GPM1a0

THE INAUGURAL RUTH GALL MEMORIAL LECTURE

On 8 March 2018 we held the inaugural A/Prof. Ruth Gall Memorial Lecture which was given by Prof. Jennifer Martin from Griffith University to mark International Women's Day. Ruth was the first woman to Head the School of Chemistry at the University of Sydney and sadly passed away in 2017. Jennifer's talk was entitled "Me and my shadow CV" and covered aspects of her career in the sciences alongside lessons learned including: the shadow CV (dealing with failure, building resilience), imposter syndrome, and the volatile and uncertain world (the need for diverse teams). We were joined at the lecture by Ruth's family and unveiled a portrait of Ruth painted by local artist Dr Kate Gradwell which will hang in Lecture Theatre 3 in the School of Chemistry.

Professor Jennifer Martin

Dr Kate Gradwell (L) with Judy Gordon (R), Ruth Gall's niece

GRADUATES OF 2017

BACHELOR OF SCIENCE (ADVANCED) WITH HONOURS

The following students had their degrees awarded in 2017:-

Mr James Batten

Nontoxic metal-cyclam complexes: Synthesis, structure and activity against mycobacterium tuberculosis

Research supervisors: Associate Professors Peter Rutledge and Mat Todd

Mr Timothy Cashman

Targeting prostate cancer with a Pt(IV) complex

Research supervisor: Professor Trevor Hambley

Mr Bowen Ding

Study into localised through-space inter-valence charge transfer in metal-organic frameworks

Research supervisors: Associate Professor Deanna D'Alessandro and Professor Cameron Kepert

Mr Xiaofan Jiang

Design and synthesis of multi-armed cyclams as novel chemical probes for studying amyloid-β (Aβ) aggregation

Research supervisor: Associate Professor Mat Todd

Ms Ayla Jones

Light-activated polypyridyl ruthenium prodrug for tuberculosis

Research supervisors: Associate Professor Siegbert Schmid and Professor Adam Bridgeman

Mr Phillip Karpati (University Medal)

Selenium-mediated peptide ligations at proline-proline junctions

Research supervisor: Professor Richard Payne

Mr Paul King

Oxa-Pictet-Spengler reaction: Mechanism and catalyst leads

Research supervisor: Associate Professor Mat Todd

Ms Heather Lacey

The secondary metabolites of novel fungal species Aspergillus nanangensis

Research supervisors: Associate Professor Peter Rutledge and Dr Rob Baker

Ms Kate Leslie (University Medal)

Expanding the scope of naphthalimide fluorophores

Research supervisors: Professor Kate Jolliffe and Associate Professor Liz New

Ms Linda Mitchell

Development and study of fluorescent probes for platinum complexes

Research supervisors: Associate Professor Liz New and Professor Trevor Hambley

Mr Andrew Roxburgh

Structural and physical characterisation of perovskite related ionic conductive materials

Research supervisor: Associate Professor Chris Ling

Mr Matthew Roxburgh

Integrating multiple functions into spin crossover framework materials

Research supervisor: Professor Cameron Kepert

Mr Arthur Tang

Design and synthesis of gallinamide A analogues as potent antimalarial drug leads

Research supervisor: Professor Richard Payne

BACHELOR OF SCIENCE (HONOURS)

The following students had their degrees awarded in 2017:-

Mr Takanori Hioki

Tricyclic acetamide ligands targeting the translocator protein as biomarkers of neuroinflammation

Research supervisor: Professor Michael Kassiou

Mr Jun Ki Hong

Nanoscale understanding of halogen bond driven self-assembled perfluorocarbon monolayers on silicon

Research supervisor: Associate Professor Chiara Neto

Mr Shuai (Gavin) Huang

The Chin action formalism of Feynman's path-integral description of quantum mechanics

Research supervisor: Associate Professor Meredith Jordan

Mr Poya Kavianpour

Borinostat: A new class of boron histone deacetylase inhibitors

Research supervisor: Professor Lou Rendina

Ms Rebecca Lee

Boronic acid and carborane derivatives of cyanine dyes

Research supervisor: Professor Lou Rendina

Ms Amy Robertson

Gadolinium rhodamine complexes as mitochondrial theronostic agents

Research supervisor: Professor Lou Rendina

Mr Jyah Strachan

Studies of sustainable catalysis using metal nanoparticles

Research supervisors: Professor Thomas Maschmeyer and Associate Professor Tony Masters

Ms Claire Wallace (University Medal)

Magnetic circular dichroism in supramolecular complexes

Research supervisor: Dr Girish Lakhwani

Mr Cameron Ware

Fabrication and characterisation of slippery lubricant infused polymeric wrinkled surfaces

Research supervisor: Associate Professor Chiara Neto

Mr Hunter Windsor

Spin crossover and redox activity in tetrazine-based metal-organic frameworks

Research supervisors: Associate Professor Deanna D'Alessandro and Professor Cameron Kepert

Ms Michelle Yu

Thermal diffraction studies of rhenium and technetium compounds

Research supervisor: Professor Brendan Kennedy

BACHELOR OF SCIENCE (ADVANCED MATHEMATICS) WITH HONOURS

The following students had his degree awarded in 2017:-

Mr Marcus Graziotto (University Medal)

Investigating the biological activity of platinum complexes

Research supervisors: Associate Professor Liz New and Professor Trevor Hambley

BACHELOR OF SCIENCE (MEDICAL) WITH HONOURS

The following students had his degree awarded in 2017:-

Mr Christopher Brown

Target-activated metal complexes for imaging the estrogen receptor

Research supervisor: Associate Professor Peter Rutledge

Ms Angela Torrisi

Design of fluorescent ratiometric redox probes for sensing in biological systems

Research supervisors: Associate Professor Liz New

GRADUATE DIPLOMA IN SCIENCE

The following students had his degree awarded in 2017:-

Mr Sam Falvey

Cyclic derivatives of apelinergic peptides

Research supervisor: Professor Kate Jolliffe

Mr Dimitris Karis

Investigating the level of inquiry in the undergraduate chemistry laboratory in Australian universities

Research supervisor: Associate Professor Siegbert Schmid

Mr Saeel Ismail Momin

Synthesis of amphiphilic diblock copolymers for the self-assembly of multifunctional drug delivery systems

Research supervisor: Dr Markus Muellner

MASTER OF PHILOSOPHY (SCIENCE)

The following student had his degrees awarded in 2017:-

Mr Victor Akpe

Controlled, self-assembly of silica nanoparticles into uniform mesostructured glass

Research supervisor: Professor John Canning

Auxiliary supervisor: Professor Max Crossley

DOCTOR OF PHILOSOPHY (SCIENCE)

The following students had their degrees awarded in 2017:-

Dr Nabiha Elias

Design and synthesis of peptidic natural product analogues as anti-infective drug leads

Research supervisor: Professor Richard Payne

Auxiliary supervisor: Associate Professor Chris McErlean

Dr Andrew Giltrap

Total synthesis of natural products with antimicrobial activity

Research supervisor: Professor Richard Payne

Auxiliary supervisor: Associate Professor Chris McErlean

Dr Alexandra Glenister

Glucose conjugation to increase the uptake of metal complexes by cancer cells

Research supervisor: Professor Trevor Hambley

Auxiliary supervisor: Dr Anna Renfrew

Dr Mingyue Kardashinsky

Functionalised phosphonium salts for gadolinium binary cancer therapies

Research supervisor: Professor Lou Rendina

Auxiliary supervisor: Professor Michael Kassiou

Dr Jun Liang

Synthesis, characterisation, anticancer properties and biological speciation of rhodium(III)-dimethylsulfoxide complexes

Research supervisor: Professor Peter Lay

Auxiliary supervisor: Dr Aviva Levina

Dr David McDonald

Self-adjuvanting vaccine candidates for cancer and tuberculosis

Research supervisor: Professor Richard Payne

Auxiliary supervisor: Associate Professor Scott Byrne (School of Medical Sciences)

Dr Denissa Murphy

Structural investigation of electrodes for rechargeable alkali ion batteries

Research supervisor: Associate Professor Siegbert Schmid

Auxiliary supervisor: Associate Professor Chris Ling

Dr Edward O'Neill

Cobalt complexes as responsive MRI contrast agents

Research supervisor: Associate Professor Liz New

Auxiliary supervisor: Dr Paul Bonnitcha (School of Medical Sciences)

Dr Lei Qin

Squaramide-based receptors for anion recognition

Research supervisor: Professor Kate Jolliffe

Auxiliary supervisor: Professor Michael Kassiou

Dr Clara Shen

Fluorescent strategies to study the labile copper pool

Research supervisor: Associate Professor Liz New

Auxiliary supervisor: Professor Trevor Hambley

Dr Julia Wind

A combined experimental and computational approach to understanding and developing new solid-state ionic conductors

Research supervisor: Professor Chris Ling

Auxiliary supervisor: Dr Toby Hudson

Dr Qingqing Zhou

Design synthesis and biological evaluation of DYRK1A inhibitors

Research supervisor: Professor Michael Kassiou

Auxiliary supervisor: Professor Lou Rendina