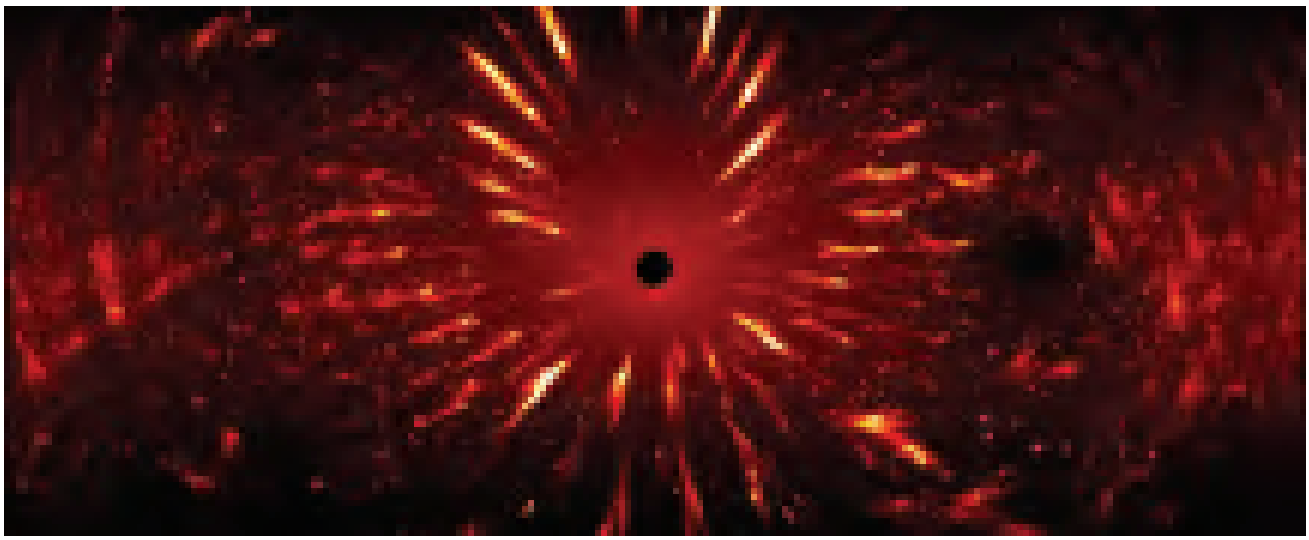
THE UNIVERSITY OF SYDNEY

2021 HONOURS PROJECTS

School of Chemistry

CONTENTS

Members of the School are active across all the traditional and emerging areas of modern chemical research. They are clustered around three multidisciplinary themes: functional energy materials; self-assembled nanomaterials; and molecular innovations in health.



FUNCTIONAL ENERGY MATERIALS

Research areas

- Molecular/ionic transport through solids
- Large-scale energy storage and conversion
- Batteries, fuel cells, selective molecular storage/separation/remediation
- Metal-organic frameworks, ionic solids, polymers, ionic liquids

Functional energy materials researchers:

- Dr Hamid Arandiyan
- Associate Professor Deanna D'Alessandro
- Associate Professor Meredith Jordan
- Dr Ivan Kassal
- Professor Brendan Kennedy
- Professor Cameron Kepert
- Professor Chris Ling
- Professor Thomas Maschmeyer
- Associate Professor Tony Masters
- Associate Professor Siggi Schmid

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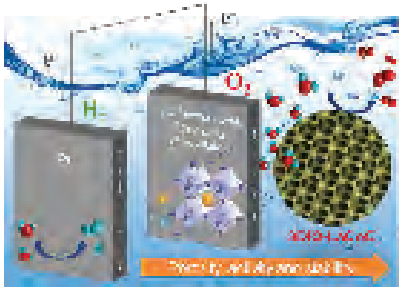
My research focuses on the solutions that aid sustainability through nano-materials design and catalytic process development. One of the main objectives of our research is to investigate rational synthetic strategies for nanocatalysts and to explore the applications of these nanomaterials in the energy and environmental sectors, such as pollutant degradation, effective energy usage, and emission control in the transportation and industry applications.

Turn "waste" into wealth: CO_2 methanation: The world is facing significant challenges, including the combination of a carbon-based energy system with the reality of global warming. The hydrogenation of CO_2 waste gas to methane (closing a loop in carbon recycling) provides an energy storage solution for intermittent renewable sources, which can be used as fuel or even as a renewable feedstock for bulk chemicals, thereby aiding sustainability. Although many efforts have been made in relation to catalytic CO_2 methanation, effectively activating the thermodynamically stable CO_2 molecule continues to be an obstacle as it requires high temperatures and is an energy-intensive process. The impasse always present regarding catalysts for energy conversion reactions is that noble metals with promising activity are limited by their high price and scarcity, whereas base metals with a lower price show more moderate performance. This project aims to investigate morphologic nanocatalysts which are low cost and show excellent CO_2 methanation efficiency. (See *Chem Comm 2018, 54, 6484; Adv. Sustainable Syst. 2018, 2, 1700119; ACS Appl Mater Interfaces. 2018, 10, 24963*). **Supervisor:** Dr Hamid Arandiyan.

Design of hierarchical nanoporous materials for energy-related application: Ordered macro- and mesoporous materials, which arose in the early 1990s, are rapidly developing as an interdisciplinary research focus. This kind of material is not only defined by a large and uniform porosity, high regularity of nanopores and large surface area but it also enables a great deal of applications by the possibilities of functional and morphological control enabled by diverse chemical compositions. A hierarchical porous material combines two or more types of pore sizes (macro-, meso- and micro-) as functional units that can meet different application requirements. For example, in a gas phase catalytic reaction, hierarchical catalysts could guarantee a good mass and flow transfer as well as avoid the pressure drop, and at the same time provide a large surface area for better activity. Therefore, the investigation of different types of hierarchical nanoporous materials for energy-related applications is highly promising. (See *Nature Comm 2017, 8, 15553; Nano Energy 2016, 27, 515; ACS Catal. 2016, 6, 6935*). **Supervisor:** Dr Hamid Arandiyan

Heterogeneous electrocatalysts for the oxygen evolution reaction: Electrocatalytic water splitting, involving a cathodic hydrogen evolution reaction (HER) and an anodic oxygen evolution reaction (OER), is an established efficient technology for hydrogen production. However, to make the electrolyser practical both reactions require an efficient catalyst to accelerate the reaction kinetics. It is particularly important to develop good anode catalysts for OER since it generally requires high overpotentials that limit the energy-efficiency of the process. (See *Nature Communications 2015, 6, 8253; Energy Environ. Sci. 2016, 9 (1), 176-183*). **Supervisor:** Dr Hamid Arandiyan



Please feel free to contact us to learn more about these and other projects availablle.

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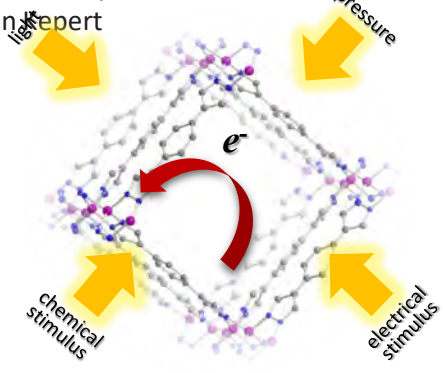
Our research spans the areas of inorganic chemistry, physical chemistry and materials science and focuses on the development of functional inorganic complexes and materials that exhibit novel electronic, optical and magnetic phenomena. Applications of our work range from the capture of greenhouse gases to address critical environmental challenges, to sensors, optoelectronics devices and catalysis for carbon dioxide conversion to fuels. A key aspect is gaining an understanding of the fundamental relationships between the structural features of the materials and their physical properties.

Project 1

Conducting Metal-Organic Frameworks (MOFs)

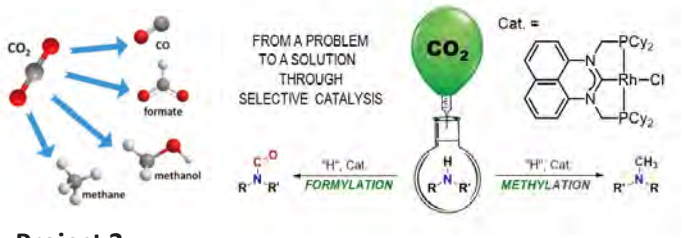
The realisation of electronically conducting microporous materials is one of the most highly sought after (yet poorly developed) goals in the field. This project will involve the design and synthesis of MOFs which exhibit stable radical states that can be generated using chemical, electrical or light as a stimulus. Solid-state electrochemistry and novel *in situ* spectroelectrochemical techniques developed in our laboratory, in addition to conductivity measurements will be employed to investigate the electronic and conductivity properties. The opportunities for advances at a fundamental and applied level are immense, with potential applications ranging from new battery materials, to lightweight sensors, and materials for energy-efficient gas separations using electrical swing adsorption. Supervisors: Deanna D'Alessandro, Cameron Kepert



Project 2

Carbon Dioxide Capture and Conversion

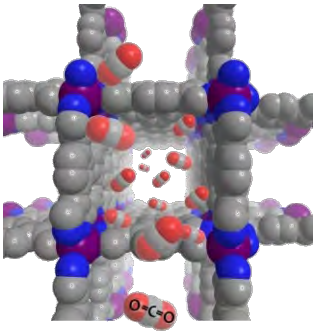
The development of more efficient processes for carbon dioxide (CO_2) capture and conversion is considered key to the reduction of greenhouse gas emissions implicated in global warming. This project is offered jointly with industry partners and will involve the synthesis of highly porous three-dimensional solids known as MOFs for use in the direct capture of CO_2 from air. A second aspect of this project is to develop and understand organometallic catalysts in order to prepare the building blocks for fine- and commodity chemicals, pharmaceuticals and fuels (i.e. methanol) from CO_2. This project may be offered jointly with Dr Indrek Pernik. Supervisors: Deanna D'Alessandro, Indrek Pernik



Project 3

Photo- and Electroswitchable MOFs

Recently, methodologies for the postsynthetic covalent functionalisation of MOFs have opened up fascinating prospects for building complexity into the pores. This project will involve the synthesis of materials as "photo- and electroswitchable molecular sieves" in which light can be used to modulate the size and electrostatic properties of the pores. This project will also make initial steps towards the integration of switchable frameworks into membranes for industrial scale processes. Supervisor: Deanna D'Alessandro



Please feel free to contact me to learn more about these and other projects available.

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We use theoretical and computational methods to examine the interactions within and between molecules in order to understand and predict chemical reactivity and the relationship between structure and function. The key to this understanding is an accurate description of molecular potential energy surface (PES). We have developed novel interpolation methods and have used them to study reaction dynamics as well as quantum effects on structure and thermodynamics.

New mechanisms in atmospheric chemistry: The predictive value of atmospheric models improves with our knowledge of the chemistry. As models become more and more accurate, it becomes more difficult to challenge their overall qualitative findings.

There are many outstanding challenges in atmospheric modelling including:

1. Only about half the observed H_2 can be accounted for by current atmospheric models. Given the increasing use of H_2 as a fuel, this is a significant shortcoming that needs to be urgently addressed. We have demonstrated a new photochemical source of H_2 although the mechanism and its ubiquity are yet to be determined.
2. In pristine environments there is a significant shortfall (by over an order of magnitude) in predicted concentrations of OH and HO_2 radicals, two of the most important radicals in the atmosphere. We have postulated novel atmospheric reactions that may produce OH and HO_2.
3. We have recently shown photochemically-induced keto-enol isomerization of acetaldehyde is a significant source of atmospheric formic acid – it is the dominant source in the marine boundary layer. We are yet to determine how important this mechanism is in other atmospheric carbonyls.
4. Reaction and collisional stabilisation of very internally "hot" atmospheric molecules, for example, after absorption of solar radiation, are complete unknowns. We propose new experiments and theory to investigate and quantify these processes.

Honours projects are available to address any or all of these challenges. They involve collaboration with experiment as well as opportunities for inter-disciplinary atmospheric box and chemical transport modelling. **Supervisors:** Associate Professor Meredith Jordan and Professor Scott Kable (UNSW – Experiment).

New methods to study gas adsorption in porous crystals: We have developed both reduced- and full-dimensional models of H_2 physisorption in metallo-organic framework materials (such as MOF-5) or carbon-based materials. Using Quantum diffusion Monte Carlo (QDMC) and Path Integral Monte Carlo (PIMC) simulations we can now determine the quantum character as well as quantum thermodynamic properties of adsorbed H_2. These techniques are also applicable to other adsorbates, e.g. CO_2 and CH_4.

Projects are available in (i) further method development: working towards new, accurate quantum methods that can be used in large, chemically realistic systems, (ii) examining temperature and gas-loading effects on adsorption and (iii) tuning adsorption enthalpy by altering the nature of the MOF and/or designing new materials for gas storage and/or separation. **Supervisor:** Associate Professor Meredith Jordan

Molecular property surfaces: We have developed new methods to describe molecular dipole moment and polarizability surfaces. These surfaces, and the molecular PES, have been used to demonstrate that the effects of both isotropic and anisotropic external electric fields (an electric field is a common model for a molecule's external environment) can be approximated using a power series expansion.

Electric fields are extremely important in biology and can change chemical structure and catalyse reactions. This project investigates the electric fields associated with the protein binding sites of neurotransmitter molecules. By making a model of the local electric field, you will be able to investigate its effects on both endogenous ligands and potential drug molecules and work towards general, transferable models for other applications. **Supervisor:** Associate Professor Meredith Jordan

Please feel free to contact me to learn more about these and other projects available.

ASSOCIATE PROFESSOR IVAN KASSAL

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We envision a world where all of chemistry can be predicted by computers. Toward that goal, we develop theoretical and computational tools to better understand fundamental chemical processes and to design superior devices, especially solar cells. One focus in our group are energy and charge transport, which underpin photosynthesis, solar cells, batteries, and molecular electronics.

We values openness, integrity, clarity, rigour, collaboration, and diversity. Our Honours students at USyd have solved some of the most important problems in our field, and they have all won University Medals. Being theorists, we were not slowed down by COVID, but became experts in remote work, and we welcome students unable to attend USyd in person. No programming experience is necessary to join us, only a willingness to learn.

Chemical Reactions on Quantum Computers

We've shown that quantum computers could solve chemical problems much faster than conventional computers. As a result, chemistry is seen as a killer app for quantum computers, targeted by all the major players in the quantum industry. This project is part of our effort, with colleagues in Physics, to demonstrate the first simulation of a chemical reaction on a working quantum computer. You will use theory and simulation—or even a real quantum device—to discover ways to map chemical reactions onto quantum computers, interpret experimental results, and overcome the limitations of existing quantum hardware. All along, you will also be paving the way for the first practical application of quantum computers.

This project can be co-supervised with Prof. Michael Biercuk, or undertaken by students in Physics.

Simulating Organic Electronics

Organic semiconductors can be made into light-emitting diodes for displays and lighting, photovoltaics for truly green energy, and transistors for flexible electronics. Despite their successes, elementary processes in these materials are poorly understood. This project will develop fundamental new theories to describe charge and energy motion in organic electronics, so that rational design can replace the current trial-and-error approach. A possible focus will be on relating device-scale performance with intrinsic molecular disorder.

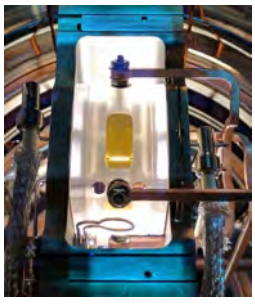
A project combining theoretical prediction and experimental tests is also possible, co-supervised with Dr. Girish Lakhwani.

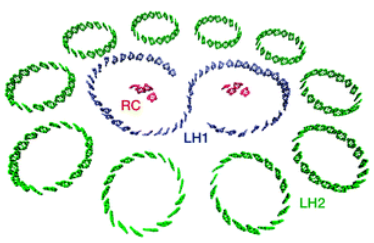
Bio-inspired & Quantum-enhanced Light Harvesting

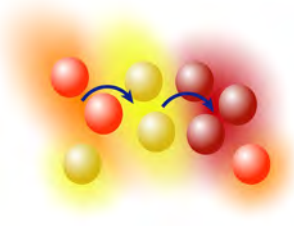
We've shown that photosynthetic organisms use quantum effects to improve their light harvesting. However, quantum improvements in light-harvesting have never been demonstrated conclusively because no one has found a way to turn coherence on and off. In this project, you will use ideas about quantum control to design a proof-of-principle device with dramatically quantum-enhanced light harvesting. You will also work with experimentalists to turn your predictions into reality.

Please contact me for details and about research areas on our group website, www.kassal.group

Figures (L to R): Ion-trap quantum computer we work with; photosynthetic light-harvesting apparatus of purple bacteria; charge transport in organic semiconductors; out having fun.







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In the Kennedy lab, we study the relationships between chemistry, crystal structure, and electronic and magnetic properties of non-molecular solids. We make extensive use of landmark Synchrotron and Neutron Facilities in addition to the state-of-art facilities at the University of Sydney.

The role of oxide conductors a low carbon economy

Solid Oxide Fuel Cells have the potential to be the ultimate low carbon energy source; This work is concerned with the development of stable oxide conducting membranes, that would separate the active anode and cathode in a fuel cell. Such membrane must have low electrical conductivity and high oxide conductivity. This project will explore the use of non-stoichiometric oxides for such applications.

Structural and Magnetic Phase Transitions

Double perovskites ($A_2BB'O_6$) serve as an ideal framework to study magnetic interactions between different transition metal ions, due to the variety of virtual electron transfers between overlapping metal orbitals which can take place through the ligand (superexchange interactions). We have recently shown that the heavier (5*d*) transition metals have unique magnetic properties and this project seeks to increase the number of examples.

Using Oxides as hosts for toxic metals

Although heavy metals occur naturally throughout the earth's crust, human exposure to these has risen dramatically as a result of an exponential increase of their use in industrial, agricultural, domestic and technological applications. Most environmental contamination and human exposure results from anthropogenic activities such as mining and smelting operations, industrial production and use, and agricultural use of metals and metal-containing compounds.

This project uses crystallographic knowledge to reverse engineer oxides capable of selectively binding heavy metal.

What are the minerals on Saturn's moon Titan?

The Cassini spacecraft has revealed Saturn's largest moon Titan to be a diverse world, with geological features that are astonishingly similar to those found on our own world. But what are the surface materials? Photochemical processes in Titan's atmosphere are driven by solar radiation and energy from Saturn's magnetosphere. Under these processes, nitrogen and methane dissociate into radicals and then recombine, generating organic molecules that range from simple (ethane, acetylene and hydrogen cyanide) to more complex molecules. It is these that make up the surface, but very few of the molecules calculated to exist on Titan have been fully characterised in their solid state.

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Six projects are available, with points of focus spanning a broad range of topics and techniques.

Electronic switching: This project involves the synthesis and characterisation of nanoporous molecular hosts that switch electronically due to the presence of spin centres within their frameworks. In generating the first materials of this type, we have recently discovered a wide range of completely new materials properties in which the switching and host-guest behaviours are linked. The global vision of this work is the generation of materials for device-application where switching acts as a mechanism for data storage, sensing, molecular recognition and molecular control. **Supervisor:** Professor Cameron Kepert.

Negative thermal expansion (NTE): The decrease of crystal lattice dimensions with increasing temperature (NTE) is a potentially useful property that has been observed only very rarely. This project will involve the use of X-ray and neutron diffraction to characterise the effect in selected framework materials. Chemical modification by doping will be investigated in an attempt to develop crystals displaying zero thermal expansion. **Supervisor:** Professor Cameron Kepert.

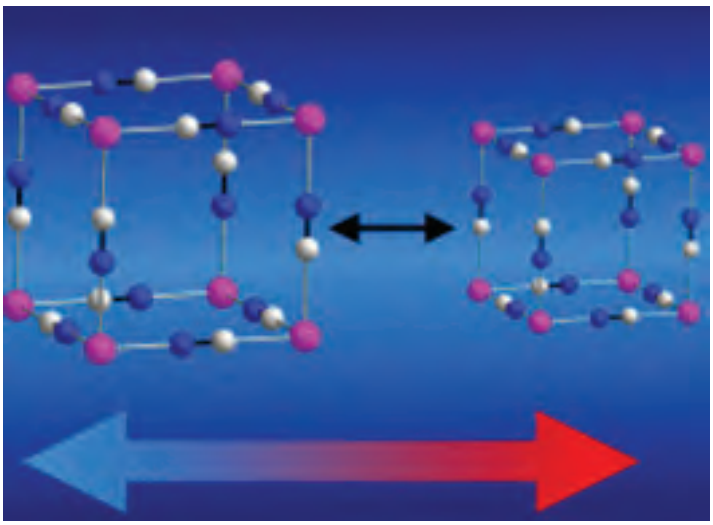
Guest desorption and adsorption: Nanoporous molecular framework materials have recently been shown to remain crystalline following guest desorption. In this project, single crystal X-ray diffraction will be used to characterise both the removal and re-introduction of guest species within molecular host lattices. Primary aims are towards understanding the structural features that lead to nanoporosity and, more fundamentally, how molecular hosts respond to the presence of guests (and vice versa). **Supervisor:** Professor Cameron Kepert.

Nanoporous chiral frameworks: The recent discovery of molecular materials that are both nanoporous and homochiral paves the way for unique approaches to enantioseparations. This project extends this important discovery by investigating the synthesis and guest-exchange chemistry of new chiral materials. Experiments into the selectivity of these processes will be fundamental in evaluating the suitability of the materials for commercial application. **Supervisor:** Professor Cameron Kepert

Hydrogen storage: In the proposed Hydrogen Economy, hydrogen gas replaces fossil fuels at the centre of a clean energy cycle. This project will address the safe and efficient storage of hydrogen gas – one of the principal current challenges in this area – through the use of nanoporous phases designed to have high surface areas and functionalised chemical surfaces. **Supervisor:** Professor Cameron Kepert.

Redox-active molecular frameworks: This project will involve the use of redox-active species to construct nanoporous framework materials with novel electronic and magnetic properties. Particular aims of the project are the synthesis of nanoporous magnets and electrically conducting nanoporous materials. *This project is in collaboration with Associate Professor Deanna D'Alessandro.* **Supervisor:** Professor Cameron Kepert.

Please feel free to contact me to learn more about these and other projects available.



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The goal of our research is to discover, characterise and optimise functional solid-state materials. We take a "crystal chemical" approach whereby we relate the crystal structure of a material to its chemical composition on the one hand, and to its physical properties on the other, to guide the design and synthesis of improved materials.

Energy materials
Project 1: Surprising and (potentially) useful magnetism in lithium-ion batteries
Despite the huge amount of interest in battery materials, very little is known about their low-temperature magnetic properties. These are not only a "gold mine" of fundamentally interesting research, but a promising means of characterising the Li content at any point in the charge-discharge cycle. This project will involve synthesis, modification (e.g., ion-exchange), magnetic measurements, neutron diffraction, building and testing batteries.

Supervisor: Professor Chris Ling

Energy materials
Project 2: Mixed ionic-electronic conductors
Mixed ionic-electronic conduction (MIEC) is a rare property required for fuel-cell electrodes. We recently discovered a number of new MIEC oxides following the key breakthrough of growing cm-sized single crystals in our floating-zone furnace (FZF). This project will investigate new barium-based oxides predicted to show MIEC, with FZF crystal-growth as a centrepiece. We will use the crystals for physical property and neutron spectroscopy experiments, supported by *ab initio* (DFT) dynamics calculations.

Supervisor: Professor Chris Ling

Multifunctional materials
Project 1: Using high-pressure to shorten and strengthen metal-metal bonding
Negative thermal expansion, where a material expands on cooling, can arise through a range of mechanisms. We recently discovered a new class that seems to work by forming unusual metal-metal bonds. The goal of this project in to design and synthesise new compounds in this class and understand how they work. It will use high-pressure/high-temperature synthesis to stabilise them, low-temperature (<0.1 K) physical property measurements and synchrotron X-ray methods.

Supervisor: Professor Chris Ling

Multifunctional materials
Project 2: Naturally layered multiferroics – combining properties on an atomic scale
Multiferroics exhibit both ferroelectricity (electrical polarisation) and ferromagnetism (spin polarisation). They have important applications as sensors, actuators and – potentially – data storage media. This project will use naturally layered ferroelectrics as "templates" for atomic layers of magnetic cations. It will involve: DFT calculations to predict the stability of new compounds; controlled-atmosphere reactions; neutron and synchrotron diffraction; magnetic and electronic property measurements.

Supervisor: Professor Chris Ling

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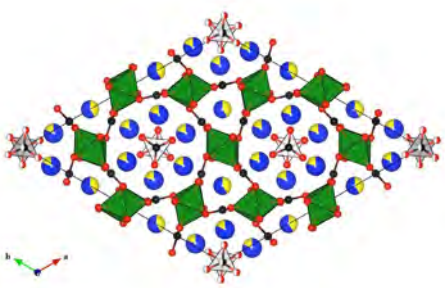

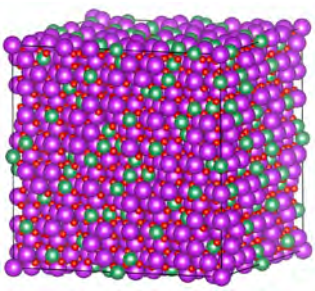

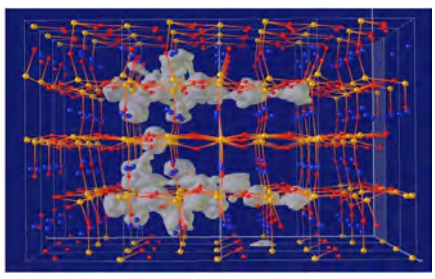

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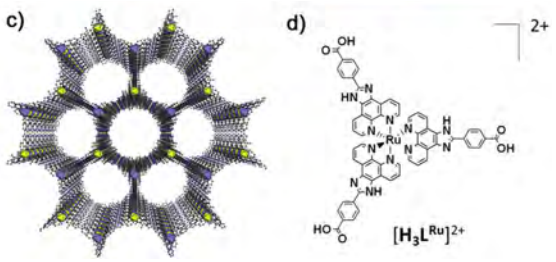
Our research area uniquely encompasses both organic and inorganic chemistry to develop interesting functional porous materials for hydrogen generation, storage and transport, amongst other energy driven applications. Using diffraction methods from the Australian Synchrotron, we are able to piece together the structure-function relationships of these new materials and continually refine them for better performance.

Skills acquired from these projects include:

X-ray single crystal and powder diffraction, synchrotron diffraction, organic synthesis and MOF characterisation using NMR, UV-Vis and gas adsorption.

Photoactive frameworks for water splitting or CO_2 reduction

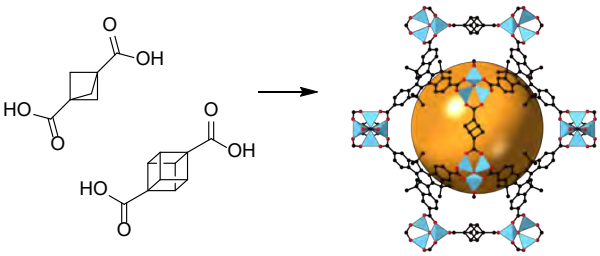
Luminescent MOFs (LMOFs) are rapidly gaining interest due to their promise in a broad range of applications including chemical sensing, artificial photosynthetic catalysis and optoelectronics. Recently, we have found tuneable luminescence can be gained through modulation of linkers with mixed functionalities and the incorporation of mixed metals. This project investigates increasing the luminescent lifetimes of phenanthroline based MOFs through varying the conjugation in the MOF linker. Supervisors: Lauren Macreadie and Deanna D'Alessandro (collaboration with Uni Otago in NZ).



Aliphatic frameworks for hydrogen and CO_2 storage

Most MOFs are constructed using aromatic linkers, such as terephthalic acid (H_2bdc), due to their low cost and well understood chemistry. Consequently, over 10,000 MOFs are made with only H_2bdc, giving a very poor representation and understanding of aliphatic based systems. Our team works with rigid, aliphatic linkers such as cubane-1,4-dicarboxylic acid (H_2cdc) and have discovered enormous potential in these systems. Due to the bulky nature of the cubane, more supramolecular interactions are possible between the host and guest systems. This project extends the investigation to other aliphatic linkers which will exhibit exciting properties. This is a high impact project and involves the investigation into the different host-guest behaviours between aliphatic and aromatic MOFs.

Supervisor: Lauren Macreadie

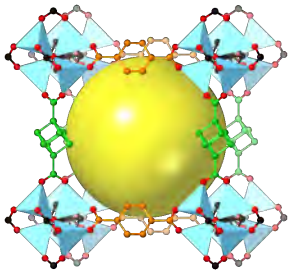


Negative thermal expansion (NTE) of aliphatic MOFs

Many materials exhibit positive thermal expansion with temperature. However, MOFs interestingly exhibit negative thermal expansion (NTE) – a phenomenon not often seen in materials. This is advantageous when trying to design zero thermal expansion materials which are highly sought after in industry. MOFs exhibit local twisting vibrations around the metal clusters and long-range translational motion of the linkers upon heating, however these responses still need to be verified in aliphatic MOF materials. This project will tune the NTE coefficient in MOFs through varying the aliphatic to aromatic linker ratio, followed by careful investigation using powder X-ray diffraction is used at both the Australian synchrotron and the Wombat diffractometer at ANSTO.

Supervisors: Lauren Macreadie and Cameron Kepert

Please feel free to contact me to learn more about these and other projects available.



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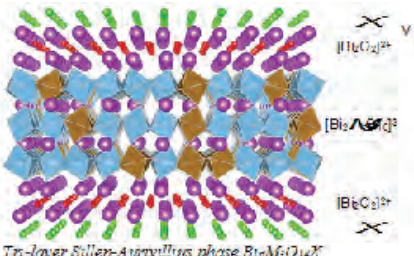
Our research aims to enhance sustainability by generating and using new fundamental insights on the molecular and nanoscopic level to develop feasible leads for the design of new catalytic chemical routes and processes. For us to even approach a "sustainable" existence, such that the ecosphere exists in a "steady state" able to support our current lifestyle, a 4- to 10-fold increase in the resource efficiency of existing production processes is necessary. Our group offers the following projects around this theme.

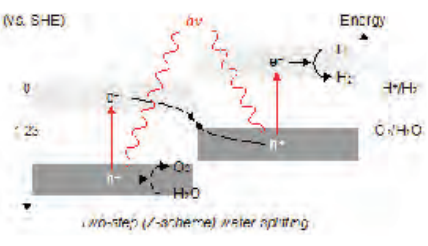
Next-generation composite photocatalysts for solar energy capture: This project aims to prepare new photocatalysts that capture and convert solar energy to stored energy by directly splitting water into oxygen and hydrogen, a perfectly clean and renewable fuel. The project will use a "bottom-up" nanoscale approach, in which compounds (such as perovskites and transition metal nitrides) with different chemical and electronic properties, but with compatible crystal structures in at least one dimension, are assembled in a single synthetic step to form a well-ordered composite. By making composites of compounds the band gaps - crucial to capturing light - and surfaces -crucial to evolving hydrogen and oxygen gas- of which complement each other, the project aims to deliver higher performing materials at a lower cost than can be achieved by conventional top-down modification. The goal of this project is to use fundamental insights from defect engineering and rational crystal-chemical design to synthesise new materials from complementary components that exhibit the desired properties, thereby yielding more effective overall solar photocatalytic water splitting catalysts. *This project may be offered jointly with Prof Brendan Kennedy or A/Prof Chris Ling.* **Supervisor:** Prof Thomas Maschmeyer.

Biomass waste for a renewable future: The Chemical Industry is highly reliant on aromatic chemicals for the production of plastics, textiles, pharmaceuticals and agrochemicals, etc. These are currently sourced from dwindling fossil reserves. Lignocellulosic (woody) biomass is the largest source of renewable aromatic species in the form of lignin: the aromatic polymer component of wood that is responsible for a large portion of its structural strength and durability. This project will synthesize non-precious metal carbide and nitride composite catalysts for the reductive conversion and upgrading of (waste) lignin to useful aromatic chemicals. Potential research avenues involve the use of the synthesised catalysts with supercritical solvents (high-pressure chemistry in batch reactors) or as novel electrode materials for electrochemical hydrodeoxygenation. Analyses of model systems using low molecular weight biomolecules (alcohols, ketones, sugars, etc) will also be used to elucidate reaction pathways and evaluate and catalytic performance. *This project may be offered jointly with A/Prof Tony Masters and Dr Alex Yuen.* **Supervisor:** Prof Thomas Maschmeyer.

State of the art magnesium batteries: This project aims to build a safe, scalable as well as high power and energy density magnesium battery with potentially twice the energy density of the current best commercial batteries. By harnessing the power of self-assembly and using mechano-chemical syntheses, novel battery materials will be prepared and used for the fabrication of electrodes. In conjunction, safer and better performing non-Grignard-based electrolytes will be prepared. Testing and optimisation of these new and integrated materials in coin cell assemblies will then form the basis of fundamental studies into the way these batteries operate and direct optimisation studies to improve Mg-battery performance. *This project may be offered jointly with A/Prof Tony Masters and Dr Alex Yuen.* **Supervisor:** Prof Thomas Maschmeyer.

Please feel free to contact me to learn more about these and other projects available.





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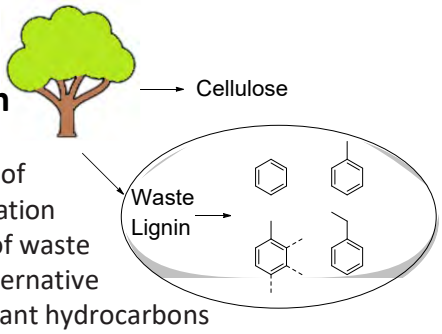
Our research is aimed at increasing resource efficiency of existing processes and the invention of novel catalysts for industrial chemical transformations. For example, fundamental studies of workhorse reactions, such as catalytic hydrogenations and improved catalysts for hydrocarbon oxidations. In the energy sphere, we are developing magnesium batteries and hydrogenase mimics for hydrogen production.

Valorisation of Lignin

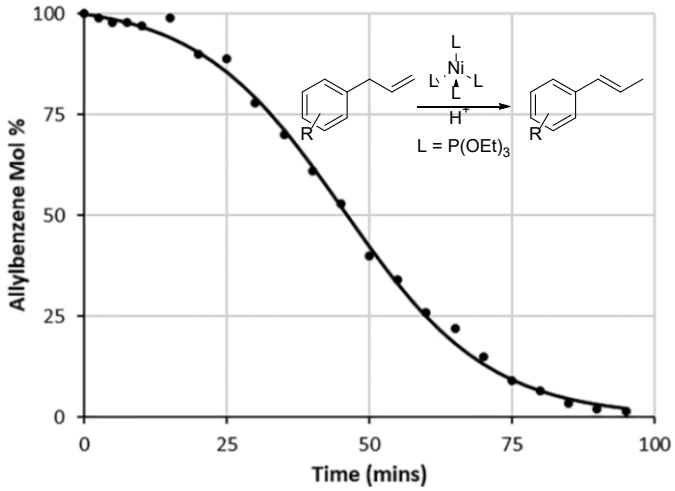


Lignin is a major (and underutilised) component of biomass. The depolymerisation and hydrodeoxygenation of waste lignin would provide an alternative source of industrially relevant hydrocarbons and divert a waste stream into valuable materials.

This process has been done successfully using supercritical conditions, though not with mild conditions. This project aims to develop a flow-electrocatalytic route to convert lignin derivatives to BTEX in high yield and selectivity under mild conditions. *This project may be offered jointly with Prof Thomas Maschmeyer, Dr Alex Yuen, and Dr Christopher Barnett.* ***Supervisor****: A/Prof Anthony Masters*

Nickel Catalysed Olefin Isomerisation

The isomerisation of aryl olefins using the precatalyst $Ni(P(OEt)_3)_4$ presents as autocatalytic. The mechanism and scope of this rare reaction type are not yet fully understood. An opportunity exists to learn a wide variety of techniques including synthesis, air-sensitive chemistry, complex analysis, and modelling. *This project may be offered jointly with Prof Thomas Maschmeyer, Dr Alex Yuen, and Dr Christopher Barnett.* ***Supervisor****: A/Prof Anthony Masters*

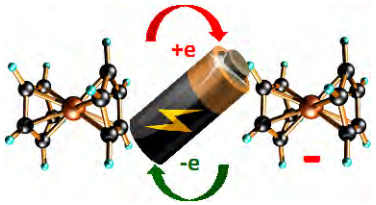


Ferrocene-based Battery–Supercapacitor hybrids

Ferrocene, the archetypical metallocene, was first reported in 1951. Since its discovery, ferrocene has been the subject of an enormous amount of study but has found few real-world applications. Stable, cheap, long life batteries and super-capacitors are the key to the roll-out of renewable energy technologies. Building on our extensive expertise in metallocene synthesis and in collaboration with industry, this project will involve the synthesis of novel ferrocene derivatives, their incorporation into half cells and batteries and evaluation of their performance as part of the new generation of energy storage devices.

This project may be offered jointly with Prof Maschmeyer, Dr Alex Yuen and Dr Max Roemer.

Supervisor*: A/Prof Anthony Masters*

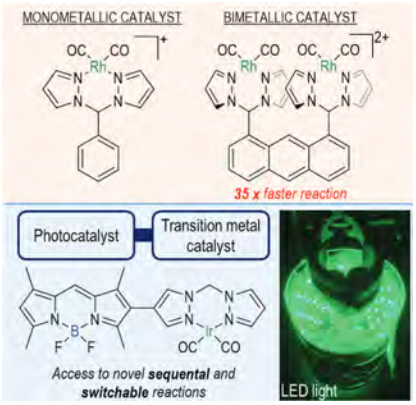


Bimetallic catalysis

The hydrogenase enzymes, with iron and nickel at their active sites, are able to perform hydrogenation far more efficiently than any man-made process to date. This project aims to synthesise functional models of bio-inspired catalysts to hydrogenate and interconvert H_2 to H^+.

This project may be offered jointly with Prof Thomas Maschmeyer, Dr Alex Yuen, and Dr Christopher Barnett. ***Supervisor****: A/Prof Anthony Masters*

An approach to accessing efficient catalysts is by designing these scaffolds so that they can host two metals simultaneously. Having two metals in close proximity to each-other (ca. 3.5 Å), has been shown to significantly improve the catalytic activity. However, in many cases the reasons for this enhancement are not straight-forward, and this enhancement can be significantly greater than predicted. Our work is concentrated on investigating the individual design effects to understand the factors that provide the optimum beneficial cooperative effects. *Collaboration with Dr Indrek Pernik and Dr Max Roemer* ***Supervisor****: A/Prof Anthony Masters.*



Please feel free to contact me to learn more about these and other projects available.

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My research interests are both in Chemistry Education and Functional Materials Chemistry. Chemistry Education research projects are designed to improve our understanding of how we best support student learning, in the widest possible sense. My group also focuses on developing novel and improved ceramic materials for use in a range of technological applications.

All projects on offer are student-centred, i.e. the direction these projects take will be based on your interests and strengths.

Inclusive Learning by Design

At the School of Chemistry, we aim to build an inclusive culture for staff and students. We have embraced changes in the undergraduate curriculum that offer diverse pathways for science students.

Projects in this domain will develop, for example, experimental procedures that allow students who are blind or low vision, to work in the laboratory independently and empower them to be active participants in their learning. Further projects can be designed with interested students.

Assessment Design

With increased emphasis on graduate qualities @Sydney and nationally, and moving from aspirational to verifiable, it is essential that we confirm that our assessments are fit for purpose or adapt them if they are not. We developed a framework to do this in straightforward fashion.

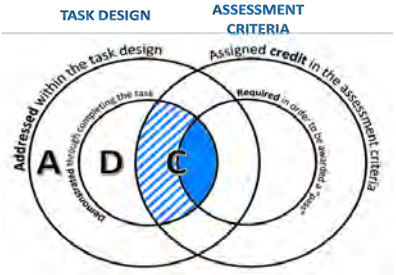


Figure 1. Two parts assessment: Is the targeted learning outcome covered in the assessment (you would hope so!), and is it weighted heavily enough in the marking scheme to confirm attainment of it? Applying this scheme will allow you to classify assessments and in doing so, important lessons can be learned for assessment design.

Supervisor: A/Prof. Siggi Schmid with other members of the Chemistry Education and Communication Research Theme

Sustainable energy storage

Rechargeable lithium ion batteries are widely used in portable electronics and hybrid or electric vehicles. Also, producing energy through sustainable means requires cheap and efficient storage to maximise the benefits. Compounds that can reversibly insert lithium have potential to be used in rechargeable lithium ion batteries. Our current program looks at a range of suitable compounds from defect perovskites to spinels and olivine type structures. This project aims to synthesise target compounds and to examine their chemical and electrochemical lithium intercalation behaviour. The products will be examined using X-ray and neutron diffraction at both national and overseas facilities.

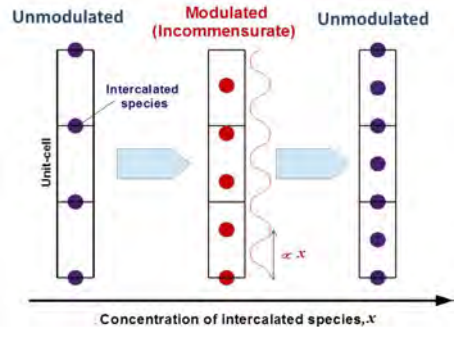
This project is in collaboration with Professor H. Ehrenberg, KIT, Germany and Dr William Brant, Uppsala University, Sweden.

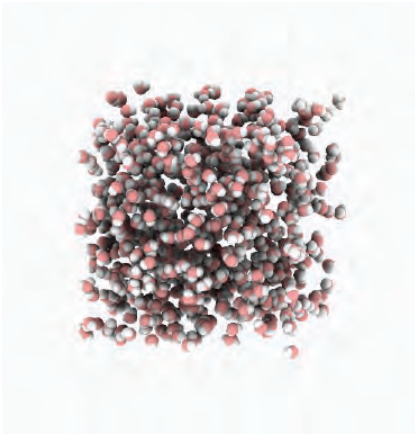
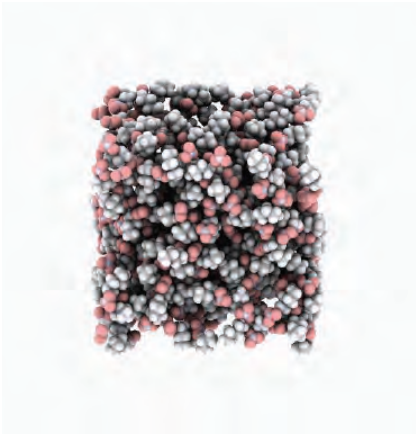
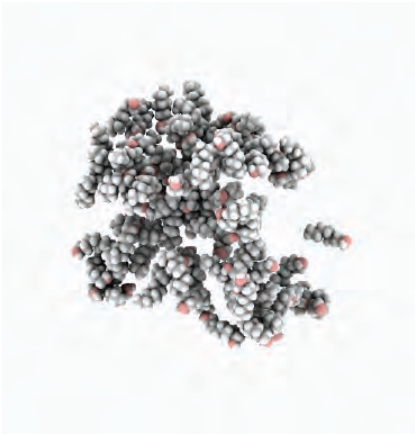
Supervisor: A/Prof. Siggi Schmid.

Modulations and other Challenges

Electrode materials in rechargeable Li- or Na-ion batteries, that follow a solid-solution mechanism, change composition over very large ranges while maintaining their structure type. This is reminiscent of compositionally and displacively flexible systems that form incommensurate composite structures. While the compounds exist in 3D, their structure descriptions need higher dimensional space. Is that for you?

Figure 1. Schematic of electrode, with changing lithium concentration. Lithium ions are located where the modulation function (vertical centre) has its maxima.



SELF-ASSEMBLED NANOMATERIALS

Research areas

- Nanoscale interactions in materials and interfaces
- “Smart” energy-efficient materials
- Molecular assembly in complex fluids and at interfaces
- Nanostructured functional surfaces, polymer nanoparticles and nano-systems

Self-assembled nanomaterials researchers:

- Professor Phil Gale
- Dr Toby Hudson
- Dr Girish Lakhwani
- Dr Markus Muellner
- Associate Professor Chiara Neto
- Dr Derrick Roberts
- Professor Greg Warr
- Dr Mark White
- Dr Asaph Widmer-Cooper

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Work in the Gale group on molecular recognition involves the design and synthesis of smart molecules for use as receptors, transporters or sensors for ionic (in our group frequently anionic) or neutral species. Design is at the heart of our work – we are frequently inspired by biological systems (but not limited by them), and we ultimately design and make new molecules to explore a wide range of molecular geometries and functional groups.

Electrogenic chloride selective transporters for cystic fibrosis treatment: The development of small-molecule synthetic transmembrane anion transporters for potential future use in channel replacement therapy for the treatment of diseases caused by dysregulation of anion transport such as cystic fibrosis (CF), and in treating cancer by perturbing chemical gradients within cells, thus triggering apoptosis, is an area of intense current interest. CF is a recessive genetic condition caused by dysregulation of anion transport through the CFTR anion channel in epithelial cell membranes. Chloride flux through the CFTR channel is impaired in CF, resulting in chronic lung disease in most CF patients. In this project, we will build on our work (see *Chem* 2016, 1, 127-146) to develop synthetic transporters with better chloride selectivity (over H^+/OH^-) in a biological relevant liposomal model. supervisor: Professor Philip Gale.

Intracellular organelle-specific ionophores: Synthetic anion transporters can disrupt cellular ion homeostasis and induce cell death (apoptosis), hence these drug-like molecules have been conceived as potential anti-cancer agents. More recently, a direct correlation between the cytotoxicity and increased intracellular chloride concentration mediated by synthetic anion transporters was established (see *Nat. Chem.* 2014, 6, 885-892 and *Nat. Chem.* 2017, 9, 667-675). In this project, new synthetic ionophores will be developed for targeted organelle ion transport properties to gain new insight into cellular processes induced by the ionophores. The targeting strategy is to exploit the specificity of pH and/or membrane composition in each organelles. supervisor: Professor Philip Gale.

Stimuli-responsive anions transporters for active cancer targeting: Synthetic small molecules that can carry chloride, bicarbonate or HCl across lipid bilayers are promising anticancer drugs because they can perturb ionic and/or pH gradients in cells. Toxicity to normal cells is a major concern for their therapeutic applications. In this project, you will design and synthesise anion transporters that can target cancer cells and minimise toxicity towards normal cells. Compounds contain a cleavable linkage will be designed that are originally inactive but undergo chemical transformation and become activated by cancer makers or cancer-specific environmental to facilitate anion transport in cancer cells. The project will involve organic synthesis, spectroscopic study of receptor-anion interactions, and membrane transport assays performed in lipid bilayer models. supervisor: Professor Philip Gale.

Thiourea MOFs as stimuli-responsive bulk anion transporters: Synthetic small molecule anion transporters that can carry chloride, bicarbonate or HCl across lipid bilayers are promising anticancer drugs because they can perturb ionic and/or pH gradients in cells. Toxicity to normal cells is a major concern for their therapeutic applications and can be avoided through employing transporters which can 'switch on' its activity at the cancer cell. In this project, you will design and synthesise MOFs built from anion transporters and benign transition metals. These MOFs will lock the transporters in an inactive state and are designed to 'disintegrate' in when reaching cancer cells. This will allow therapeutic targeting of cancer cells while simultaneously minimising toxicity towards normal cells. The project will involve organic synthesis, X-ray crystallography, spectroscopic study of receptor-anion interactions, and membrane transport. Supervisor: Professor Philip Gale and Dr Lauren Macreadie.

Please feel free to contact me to learn more about these and other projects available.

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The group's research involves the computer simulation of complex materials, concentrating on issues of structure and dynamics. Most of the projects involve computational experiments, but all can be done without previous experience of programming.

Predicting and designing the structures made by the self-assembly of nanoparticles into metamaterials is a key requirement for a new generation of advanced materials. Many fundamental questions are still open.

I am also interested in projects related to educational tools and knowledge representation in Chemistry.

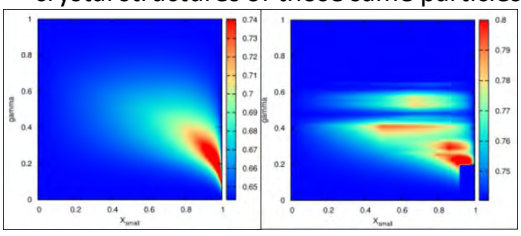
Chemistry education
Project 1. Asking unsearchable questions in chemistry.

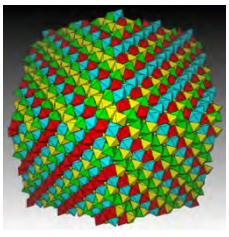
With the sudden interest in online learning and assessment due to the Covid-19 pandemic, chemistry educators across the world are rapidly designing open-book online assessments including examinations that aim to test chemistry knowledge and learning outcomes.

Most modern students are digital natives. Could they pass chemistry with Google alone? What kinds of questions most effectively differentiate between learned chemistry student and Googlebores?

Materials chemistry
Project 2. What is the connection between random packings and crystalline packings?

Jammed random packings of particles play an important role in many industrial applications including the stability of mining stockpiles, the safety of pebble bed nuclear reactors, and the stability of amorphous thin films. But there is even still wide disagreement on how to define a random packing. This project will investigate in what ways the random packings of a series of different particles are related to the ideal crystal structures of those same particles.





Materials chemistry
Project 3. Building billion year old glass in a day

Experimentalists have created a material which is extremely stable compared to normal bulk glasses, and is equivalent in most respects to a glass which has been aged for billions of years. This is done using physical vapour deposition of a warm thin film which allows molecules the flexibility to search for stable locations before they get stuck. In this project, you will simulate this process and the materials it creates.

Mathematical chemistry
Project 4. What is it about the shape of a particle that determines its packing porosity?
Some particle shapes fill space better than others, but when they self-assemble, they all try to do the best they can. In some applications this is good, and in others it is bad. Suppose you want to crystallize colloidal particles, but you want to generate a material with a high porosity. What shapes should you consider using?

We have found that particle properties like symmetries, concavity, and aspect ratio all play a role in how dense they can get. But so far we cannot explain why some shapes pack in an unusual complex pattern whereas others are quite simple.

Self assembly

Co-Supervisor: Dr Asaph Widmer-Cooper

Project 5. Porous nanoparticle superlattices for catalysis and sensing

Project 6. Phase Behaviour of Janus Rods and Helices

Please feel free to contact me to learn more about these and other projects available.

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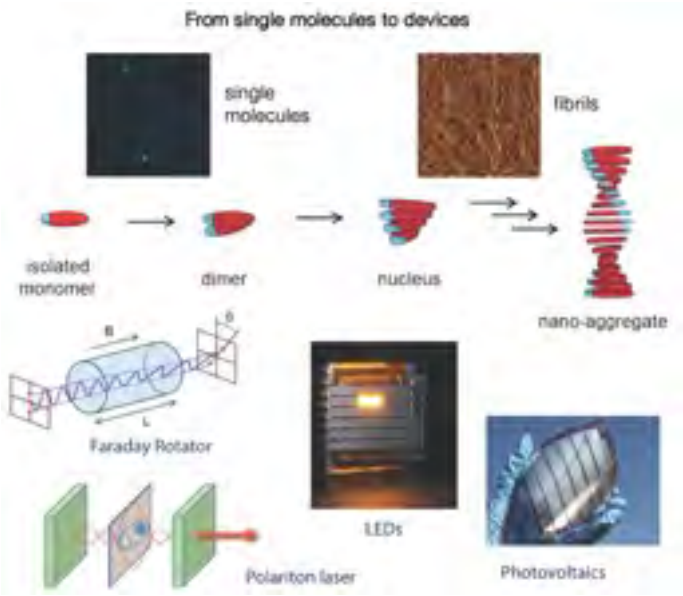
Molecular Photophysics research group is a part of the ARC Centre of Excellence in Exciton Science (ACEx), whose primary mission is to manipulate the way light energy is absorbed, transported and transformed in advanced molecular materials. Our key focus is on investigating optoelectronic properties of novel nanoscale semiconductor materials for organic solar cells, optical switches and lasers.

EXCITON SCIENCE

Studying one molecule at a time: We are heavily invested in understanding molecular parameters that underpin excitonic behaviour in a range of optoelectronic devices including LEDs, exciton logic gates and spin switches. An *exciton* is a coulombically bound electron-hole pair that is generated in a material either by light absorption or charge injection. As the size of devices decreases, single molecules dominate optical processes such as fluorescence blinking that causes emission to randomly switch on and off. In this project, we will investigate blinking dynamics in functional materials using single molecule spectroscopy and identify ways in which we can tailor this behaviour towards different kinds of device operations.



Polariton laser: Electrically injected organic semiconductor laser remains a Holy Grail in light emitting devices. Unlike conventional lasing, *polariton* lasing does not require population inversion, instead needing only strong coupling between the exciton state and a cavity photons. In this project, you will fabricate and characterise cavity devices to identify next-generation lasing materials. *A project variant involving industrial collaboration is possible.*

Organic photovoltaics: π-conjugated materials (CMs) offer cheap solution processible alternatives to silicon in organic solar cells (photovoltaics). In this project, you will fabricate organic solar cells using a range of donor and acceptor materials and geometries aimed at improving device efficiency and stability.

CHIRALITY AT A NANOSCALE

Spectroscopy using superchiral light: Detection of molecular chirality is vital for varied applications in pharmaceuticals, sensors and displays. Circularly polarised light is chiral in nature and is used to detect chiral molecules, however, the technique often fails because the light is much larger than molecular dimensions and generates a weak optical response. In this project, we will controllably generate highly twisted *superchiral* light to enhance the optical response thereby increasing the molecular footprint for high precision detection.

Chiroptical phenomena in semiconductor materials: Energy and charge transport in functional materials depend strongly on their molecular packing (also known as morphology) in thin films and nanocrystals that isn't well understood. In this project, you will perform state-of-the-art chiroptical spectroscopy experiments to characterize nanoaggregate morphology and identify structural parameters that dictate their molecular self-assembly.

We are always working on new ideas, not all are listed here. Drop me a line if you wish to know more!

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Our group is interested in finding intuitive and new ways to access unprecedented polymeric and hybrid nanostructures. Our aim is to produce multifunctional nanoscale materials for applications in catalysis, energy and nanomedicine. Polymer science provides the ideal playground for creative materials design.
You can find more information on polymer architectures and their emerging applications by browsing through our publications at polymernanostructures.com.
My team is very interdisciplinary and polymer science in general connects many areas of chemistry. As polymers find use in materials, they thus also feed into engineering and pharma disciplines. I honour the diverse interests of students and can customise research projects to specific interests or areas of application. The below provides some examples of projects currently on offer in my team.

Getting nanomaterials into shape
The application of spherical nanoparticles in biomedical fields has been studied extensively over the past decades. However, recent studies suggest beneficial interactions of non-spherical nanoparticles with biological materials and tissue. In addition, theoretical studies predict advantageous cell association for cylindrically- or disc-shaped particles. In this project, we will build on our findings and develop a new nanoparticle platform to study the efficacy and usefulness of differently shaped polymers in biomedical applications.
Supervisor: Dr Markus Müllner

Providing materials with structure
Many properties of functional materials depend critically on their effective surface areas. In this project, we will use a newly developed polymer-hybrid method to synthesise nanostructured materials with very high surface areas and very efficient internal topologies. We will target materials with applications as electrode materials in solid-state batteries and solar cells, for which nanostructuring has been predicted to enhance performance. The project will involve synthesis, characterisation on length scales from the atomic through the nanoscale to bulk surface area, and the construction of working batteries for testing under real working conditions. **Supervisors:** Dr Markus Müllner and Prof. Chris Ling

Mimicking viruses
Virus particles are multifunctional particulates allowing them to interact with cell membranes with high specificity and efficacy. Polymer science allows the synthesis of complex nanomaterials and is expected to produce synthetic versions of nature's elaborate 'cargo carrier systems'. In this project, we are investigating new means to produce functional nanoparticles capable of mimicking the properties and performance of viruses. This is collaboration with UC San Diego.
Supervisor: Dr Markus Müllner

Designing polymers through light and catalysis
In recent years, we have developed new synthetic methods to produce polymers in a more environmentally benign way by using light-induced catalysis and bismuth oxide. This allowed us to recycle catalysts, produce polymers in water, as well as enabled new polymeric hybrid materials, such as polymer-peptide conjugates in one step. This project looks at expanding the scope of this work to synthesise chain transfer agents for polymerisation that are traditionally difficult to access by conventional organic chemistry.
Supervisor: Dr Markus Müllner

Sensing made easy through polymeric scaffolds
Polymers are an attractive scaffold for responsive sensors as they can be decorated with multiple binding/recognition sites, therefore increasing the selectivity and/or binding affinity for complex analytes. This project will involve the synthesis of responsive polymers functionalised with receptors and fluorophores that can be applied to environmental or biological studies. This project will involve polymer synthesis and photophysical studies. **Supervisors:** Dr Markus Müllner and A/Prof. Liz New

Please feel free to contact me to learn more about these and other projects available.

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Our area of research is physical chemistry of interfaces, a multi-disciplinary field spanning the chemistry, physics, nanoscience and materials engineering. We focus on phenomena that occur when liquids are confined on the micro-scale, such as in microfluidics, and on designing surfaces that have advanced functional properties. Research projects are available in these areas:

Structured coatings for water capture We design polymer surfaces that collect water from the atmosphere, as part of a multidisciplinary Sydney Nano Grand Challenge project (ACWA) involving academics from across the University. The surfaces are nanostructured, highly porous polymer films, that can be applied over large areas (figure below). The produced coatings enable the delocalised collection of clean water from the atmosphere without any energy input and no moving parts. Website of ACWA: nano-acwa.sydney.edu.au; ABC The Acceleration Documentary Episode 4: https://iview.abc.net.au/show/great-acceleration/series/1/video/DO1845H004S00

Project 1

The Honours project will involve experiments relating how surface energy (chemical composition) and structure (topography, roughness) of the porous polymer coatings affects the efficiency of water collection. Data will be collected both in a controlled lab environment and on the prototype located on the roof of the SNH building.

Project 2

A second Honours project focuses on simulating water droplet roll-off behaviour over structured surfaces, using modelling software. In collaboration with Dr Asaph Widmer-Cooper.

Liquid-infused surfaces

Liquid repellence is important for energy efficiency and benefits many applications, such as self-cleaning, anti-fouling and anti-bacterial coatings. The ability for liquids to be repelled and slip over surfaces without leaving contamination behind can be enhanced if the surface has liquid-like properties, as in the figure below.

Project 3

The Honours project involves synthesising surfaces with liquid-like properties without the use of nano- and micro-structure but using liquid-like thin polymer layers grafted to a solid substrate. Part of this project could involve a synthetic component in collaboration with Dr Markus Muellner.

A new family of self-assembled monolayers

Our group has recently discovered a new family of self-assembled monolayers that form on oxide surfaces, through halogen bonding, an intermolecular interaction less known but similar to hydrogen bonding. The self-assembled monolayer effectively turns the surface properties of glass into those of Teflon and can lead to sophisticated assembly of soft matter.

Project 4

This Honours project explores the potential of these monolayers of extremely low surface energy to be used to enhance dropwise condensation.

Please feel free to contact me to learn more about these and other projects available.

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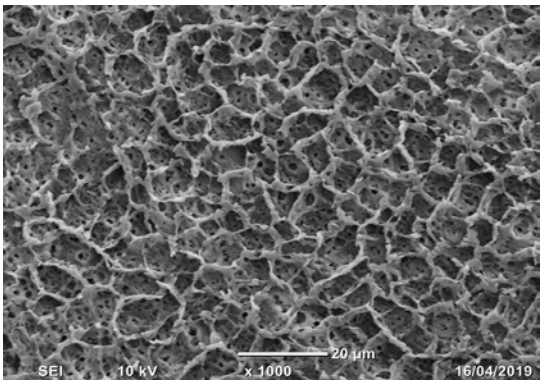
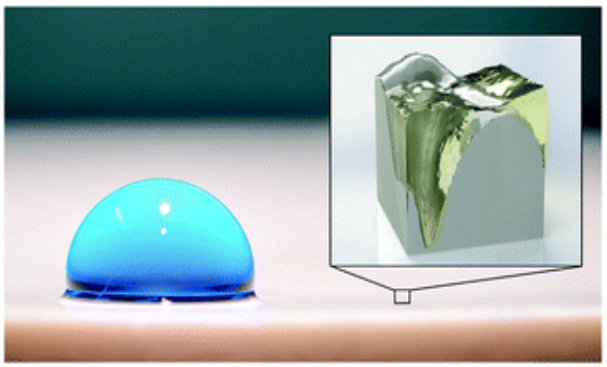
@ChiaraOz





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Our research program centres on designing self-assembled molecular materials that undergo controlled morphological transformations in response to external signals (e.g., light, pH, biochemical cues). We use supramolecular and dynamic covalent interactions to explore self-assembly phenomena spanning from small molecule recognition up to microphase separation of block copolymers, with the goal of building 'smart' nanomaterials that sense their environments and produce distinct physicochemical responses.

'Transformersomes' — shape-shifting polymer nanostructures: Amphiphilic polymers can self-assemble into an impressive spectrum of nanoscale architectures that behave in intriguing ways; from catalysis to cellular interactions. In this project, we aim to design self-assembled polymer nanostructures (polymersomes) that undergo shape transformations when exposed to light (Fig 1a). These transformable polymersomes ('transformersomes') will be able to express new physical properties in response to complex environmental changes, e.g., in living tissue during wound healing. This project will be undertaken in collaboration with Dr Markus Muellner's group. **Supervisor:** Dr Derrick Roberts.

'Clickety-Split' — click-activated self-immolative prodrugs: Prodrugs are pharmacologically inactive molecules that are converted to their active forms by biological stimuli near or at their target sites. Normal drug molecules can be converted to prodrug forms by 'capping' nucleophilic groups with "self-immolative" linkers, which are cleaved in elimination cascades resembling a burning fuse. In this project, we will develop a new type of self-immolative linker using 'click' reactions between azides and alkynes, and study their release kinetics. These linkers will then be adapted to self-immolative polymer systems for achieving intracellular drug delivery. **Supervisor:** Dr Derrick Roberts.

Dynamic-covalent metallopolymers: Metal-ligand coordination can be used to control the self-assembly of synthetic polymers into supramolecular architectures. In this project, we will prepare polymers with Schiff-base ligands that self-assemble into metallogels and helical fibrils in the presence of transition metal ions. Metallo-Schiff-base complexes can undergo dynamic-covalent exchange reactions when exposed to electron-rich amines. This property will be used to construct self-healing assemblies that can undergo stimuli-induced rearrangements through *in situ* imine exchange reactions (Fig. 1b). **Supervisor:** Dr Derrick Roberts.

Please get in touch to learn more about these and other projects available.

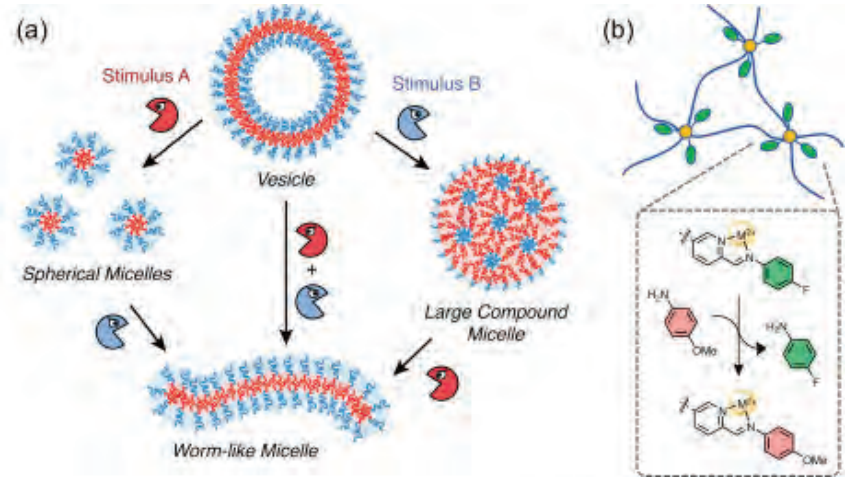

Fig. 1 (a) Transformersomes: *a proposed network of nanostructure transformations achieved through stimuli-triggered degradation of block copolymers.* ***(b) Dynamic-covalent metallopolymers:*** *dynamic imine exchange can induce stiffening of metallogel networks.*

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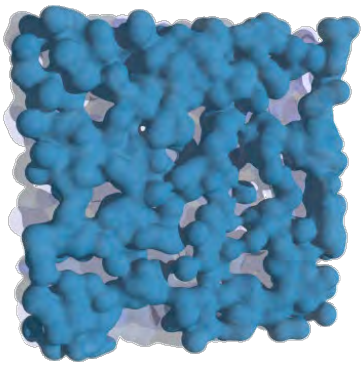
We investigate the fundamental question of how macroscopic properties emerge from the nanoscale structure and dynamics of soft matter – from ionic liquids to micelles, liquid crystals, microemulsions, biomaterials, polymers and 2D nanomaterials. We have a particular focus on ionic liquids and deep eutectic solvents as novel, nanostructured, and environmentally friendly solvents with potential for economical scale-up. Ionic liquids (ILs) are not just salts that melt at or near room temperature. They are complex, dynamic nanostructures unlike conventional molecular liquids, making them extraordinary components for as solvents for chemical reactions or formulations (see Chem. Rev., 2015*, 115, 6357.) Deep eutectic solvents are hybrid liquids that contain both ionic and non-volatile molecular components. We are exploring their nanostructure, and using this knowledge to design new kinds of soft materials. Our work makes extensive use of advanced neutron and X-ray beam techniques in our laboratory and at major international facilities, complemented by NMR, microscopy and thermal analysis.*

Soft Hybrid Nanomaterials

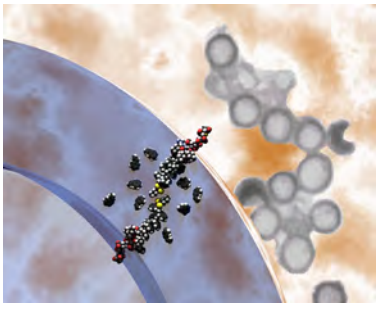
We have recently discovered new ways of making non-aqueous lyotropic liquid crystals and other nanostructured soft materials by combining concepts from self-assembly and deep eutectic solvents. This project will explore the effect of incorporating amphiphilic components like surfactants and lipids into deep eutectic mixtures to transform them from simple liquids into liquid crystals, viscoelastic gels and microemulsions. Their properties will then be explored for a variety of applications ranging from novel lithium battery electrolytes to hyperconcentrated formulations.

Self-Assembly
Micelle or nanoparticle? You be the judge.

New polymer preparation techniques allow us to move continuously in synthetic space from small, rapidly-equilibrating micelle-forming surfactants to kinetically-trapped, nanoparticle-forming amphiphilic copolymers through amphiphilic “co-oligomers.” Using stopped flow and other kinetic techniques we will explore how molecular structure affects equilibration rate of micelles, and use this to design, control and preserve nanostructure while engineering dynamics are also critical for controlled release applications for drug, perfume or nutrient delivery. (Langmuir, 2014, 30, 7986–7992).



Exobiology: Life Beyond the Goldilocks Zone



While it is widely believed that liquid water is essential for life to arise, this is an as-yet unproven conjecture. In this project we will explore which of the preconditions for life can be met in extreme and nonaqueous environments such as the ethane lakes of Titan or deep eutectic mixtures of non-volatile salts. Can we make cell membranes, and how does molecular recognition and replication operate in these environments? (Soft Matter 2017, 13, 1364-1370)

Supervisor: Professor Greg Warr

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As part of the ARC Centre of Excellence in Exciton Science (ACEx), we use computer simulations and mathematical models to understand the behavior of existing materials and to design new materials for solar energy capture, sensing, and security. Typically, this involves studying the structural and dynamic properties of complex fluids and the beautiful structures that appear spontaneously in these systems through the self-organisation of molecular and colloidal components.

Assembly of Nanorods for Solar Energy Applications

Rod-shaped nanoparticles have anisotropic optical and charge transport properties that make them attractive candidates for use in printable solar cells and luminescent solar concentrators. In this project, you will use computer simulations to study how such nanorods can be assembled into structures that are optimal for light capture and charge separation. This will yield design rules that can be used by our experimental collaborators within ACEx to create such assemblies in the laboratory.

Supervisor: Dr Asaph Widmer-Cooper

Using Molecular Hairs to Dynamically Tune Nanoparticle Properties

Ligand molecules that bind to the surface of inorganic nanoparticles are used to direct their growth during synthesis and play an essential role in keeping the particles from randomly aggregating in solution. Recently, it has become apparent that these ligands can also order on the particle surface in response to a change in temperature or solvent conditions, thus dramatically changing how the particles interact with one another (e.g. see ACS Nano 2018, 12, 5969). In this project, you will use molecular dynamics simulations and spectroscopy to investigate this order/disorder transition and how it affects the optical properties of the particles.

Supervisors: Dr Asaph Widmer-Cooper and Dr Girish Lakhwani

Formation and Stability of Printable Solar Cells

Solar cells based on metal halide perovskites represent the fastest advancing solar technology to date and have the potential to allow the manufacture of lightweight, high-efficiency cells via low-cost and energy-efficient solution processes. The efficiency of such solar cells depends strongly on the crystallinity of the films that are formed, yet we understand surprisingly little about the mechanisms by which they are formed and degraded. In this project, you will use computer simulations to study how metal halide perovskites grow and dissolve in solution.

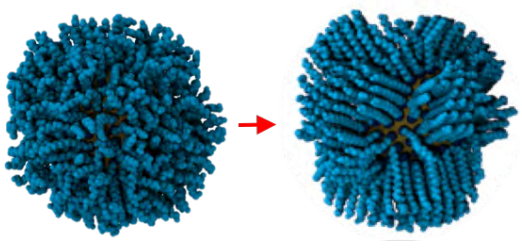
Supervisor: Dr Asaph Widmer-Cooper

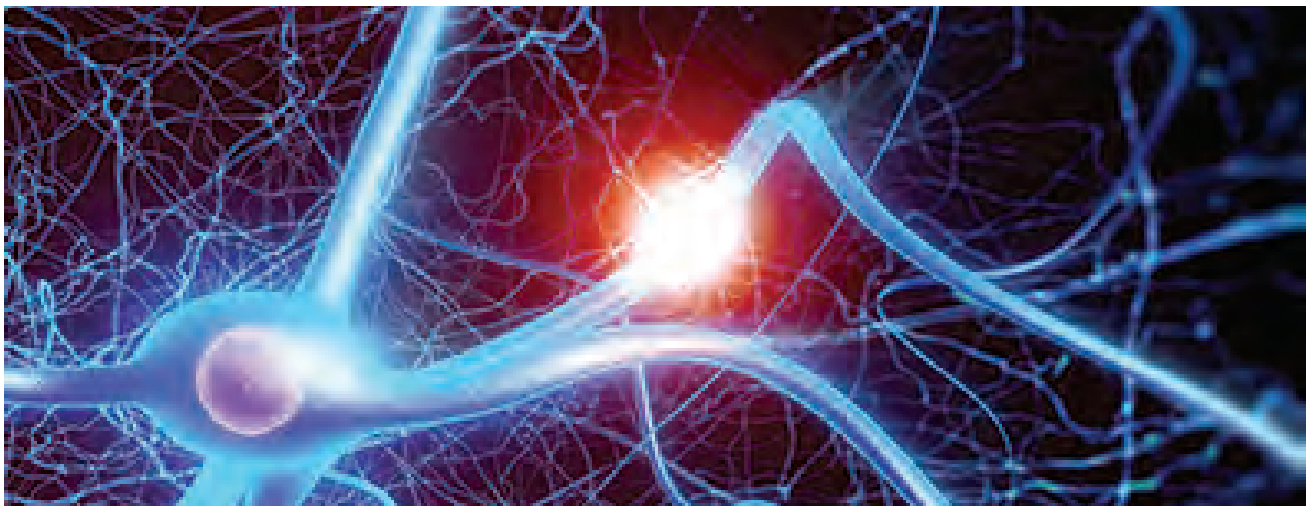
Tuning Surface Wettability and Roll-off

Being able to tune the wettability of surfaces is crucial for a wide range of applications including self-cleaning paints and water capture. Plants and insects have devised many ingenious strategies to control wettability through the use of chemical and topographical patterning. In this project, you will use computer simulations to study how surface topography and chemistry affect droplet shape and roll-off, including studying how infusing the surface with an immiscible liquid can dramatically alter these properties. This project will involve collaboration with on-going experimental work.

Supervisors: Dr Asaph Widmer-Cooper and Prof Chiara Neto

Please feel free to contact me to learn more about these and other projects available.





MOLECULAR INNOVATIONS IN HEALTH

Research areas

- Chemical signalling, neurotransmission
- Ageing, cancer, neurodegenerative diseases
- Diagnostics and therapeutics (“theranostics”)
- Drug design/discovery, biosensing/imaging, drug delivery

Functional energy materials researchers:

- Dr Samuel Banister
- Associate Professor Ron Clarke
- Dr Jonathan Danon
- Professor Kate Jolliffe
- Dr William Jorgensen
- Professor Michael Kassiou
- Dr Amandeep Kaur
- Dr Yu Heng Lau
- Professor Peter Lay
- Dr Xuyu Liu
- Associate Professor Chris McErlean
- Dr Alice Motion
- Associate Professor Liz New
- Professor Richard Payne
- Professor Lou Rendina
- Professor Peter Rutledge
- Dr Mark White
- Dr Shelley Wickham

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Our research involves the development of small molecules targeting G protein-coupled receptors and ion channels for the treatment of neurological diseases. Our interests are rare and orphan diseases not addressed by the pharmaceutical industry. Using lead structures from natural product chemical space, as well as public database mining with internally developed cheminformatics tools, we conduct lead optimisation using iterative development cycles involving molecular modelling, chemical synthesis, and preclinical pharmacology to develop clinical candidates.

Molecular medicine for mutant GABA-A receptor genetic epilepsies: A growing number of specific mutations in the subunits comprising pentameric GABA-A receptors that lead to dysfunction of the ion channel are being identified as the cause of distinct, severe epilepsy syndromes. However, many patients are refractory to multiple antiepileptic drugs

Using concatenated constructs of precisely defined GABA-A mutants in xenopus oocytes along with electrophysiology, we have demonstrated that common antiepileptic drugs are unable to restore normal functioning at these receptors. In this system, several cannabinoids restore function in at least some of the mutant receptors where other classes of clinical antiepileptics are ineffective. This project with involve the optimisation of a cannabinoid lead for potency, efficacy, and fortification against first-pass metabolism. Our optimised candidate will be screened in a mouse model of generated using CRISPR-Cas9 technology. *Collaborators include Dr. Dr Nathan Absalom (Pharmacy), Dr Michael Bowen (Psychology) and Prof. Mary Collins (Chebib) (Pharmacy).*

Phytocannabinoid derivatives as GPR55 antagonists: The cannabis plant produces more than 100 unique molecules, with two cannabinoids approved for clinical use; Marinol® for chemotherapy-induced nausea and vomiting, and Epidiolex® for Dravet syndrome. Despite the clinical utility of plant cannabinoids, the historical prohibition of cannabis has hindered research into the therapeutic potential of this diverse natural product class. We have identified several phytocannabinoids functioning as non-selective GPR55 antagonists with efficacy in mouse models of epilepsy. This project will involve the physicochemical optimisation of these cannabinoid GPR55 antagonist leads for improved target selectivity, in vivo potency, and pharmacokinetic profile. *This project is in collaboration with A/ Prof. Jonathon Arnold (Pharmacology).*

Peripherally-restricted cannabinoids ligands: Cannabinoid receptors are expressed abundantly throughout the brain, but also in the periphery. The clinically-approved cannabinoid antagonist rimonabant was withdrawn from the market owing to adverse effects associated with its central nervous system penetration (CNS), while brain-permeable cannabinoid agonists like tetrahydrocannabinol produce intoxication. By rational modification of the lipophilicity, polar surface area, and number of hydrogen bond contributors, we have developed several cannabinoid agonists and antagonists with limited ability to cross the blood-brain barrier. Peripherally-restricted cannabinoids have analgesic activity in rodents (agonists) and utility in patient-derived pluripotent stem cell models of cardiovascular and metabolic diseases (antagonists). We are developing each of these classes as new cannabinoid therapeutics with reduced adverse effect profiles. *This project is a collaboration with Dr. Thomas Wei and Prof. Joseph Wu (Stanford University, USA).*

Profiling new psychoactive substances: In the past decade, more than 450 new psychoactive substances (NPS)—novel recreational drugs created by tweaking the molecular structure of traditional drugs—have been identified as designer stimulants (e.g. N-ethylpentylone), hallucinogens (e.g. 25I-NBOMe), and cannabinoids (e.g. AMB-FUBINACA). Very little is known about the biological activity of most of these substances, and they are increasingly associated with serious adverse effects, including death. We are proactively characterising the chemistry, pharmacology and toxicology of systematic libraries of emerging NPS to facilitate early detection and mitigate harms caused by the most dangerous NPS (see *N. Engl. J. Med.* **2017**, 376, 235). The Psychoactives Surveillance Consortium and Analysis Network (PSCAN, USA) has already detected three new NPS in clinical toxicology casework using this innovative methodology. *Collaborators include Prof. Roy Gerona (UCSF, USA), Prof. Michelle Glass (University of Otago, NZ), Prof. Mark Connor (Macquarie University), and Prof. Iain McGregor (Psychology).*

Please feel free to contact Samuel to learn more! Additional details are available on our website: https://sydney.edu.au/lambert/

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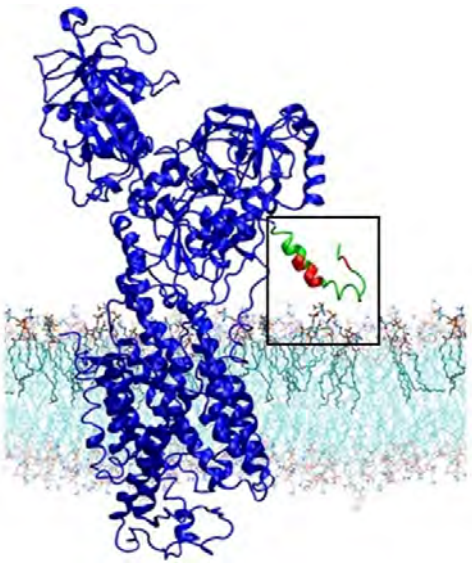
Work in the Clarke research group focuses on biological cell membranes, on the lipids and proteins of which they're composed and diseases which arise from membrane dysfunction. A particular interest of our group for many years has been ion pumps, which are involved in e.g. nerve function, muscle contraction, digestion. Our research is multidisciplinary in nature, overlapping chemistry, biology and physics.

MOLECULAR ORIGIN OF RAPID-ONSET DYSTONIA PARKINSONISM

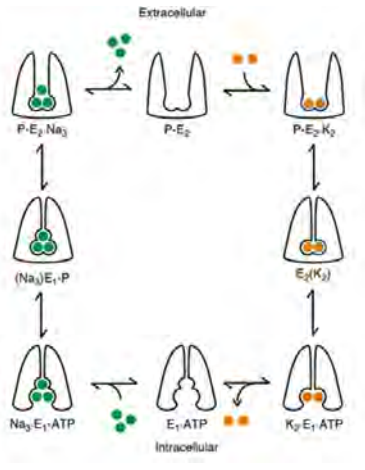
Details of project Rapid-onset dystonia Parkinsonism (RDP) is a rare form of Parkinson's disease afflicting children which is triggered by physical or emotional stress. It doesn't respond to normal treatments used in the aged, such as dopamine. The disease is caused by mutation of the α_3 isoform of the catalytic subunit of the Na^+,K^+-ATPase. The mutation causes an impairment of the enzyme's ability to discriminate between Na^+ and K^+ ions. The purpose of this project is to develop a fundamental understanding at the molecular level of the conformational changes of the Na^+,K^+-ATPase allowing it to alter its selectivity between Na^+ and K^+, and how these conformational changes are affected by mutations responsible for the development of RDP.



MEMBRANE INTERACTION OF SMALL MOLECULES CAPABLE OF ALLEVIATING BATTEN'S DISEASE (In collaboration with Dr Charles Cranfield, UTS)

Batten's disease is a hereditary neurodegenerative disease causing a disruption in lysosomal function within cells. Lysosomes are basically the cell's recycling depot. Biological molecules, which have become damaged by whatever means, are transported into the lysosome to be broken down into simpler building blocks and then returned to the cytoplasm for incorporation into new molecules. In Batten's disease this process is disrupted, causing the accumulation of waste material within the lysosome. In contrast to many other cells, the body is not able to regenerate damaged neurons, thus making the nervous system particularly susceptible. Batten's disease is caused by a mutation in the protein battenin, an integral membrane protein found in the lysosomal membrane of all eukaryotes. In 2018 it was shown that treatment of battenin-deficient mice with the sterol carbenoxolone caused a reduction in disease symptoms. This was proposed to be due to binding to the lysosomal membrane, altering its physical properties. The purpose of this project is to investigate the effect of carbenoxolone on membrane structure (e.g. fluidity, phase behaviour, electrostatics) and develop a molecular understanding of how it could benefit sufferers of Batten's disease.

Please feel free to contact me to learn more about these and other projects available.



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The goals of our research are to discover new medicines for the diagnosis and treatment of frontotemporal dementia (FTD). We use organic synthesis and medicinal chemistry expertise to design and synthesise novel therapies to combat FTD, which is a common cause of early-onset dementia and neurodegeneration. Working within this field will expose aspiring researchers to a wide variety of organic chemistry techniques, as well as enabling full participation in the early stages of the drug discovery process. The projects summarised here can be tailored to the specific interests of the participant. Jon welcomes any requests for more information.

Introduction to FTD: FTD is a common cause of early-onset dementia, with near comparable prevalence to Alzheimer's disease (AD) for 45-55-year-olds. Diagnosis is complicated due to its shared clinical and pathological features with related neurodegenerative disorders such as motor neurone disease (MND). FTD is characterised by rapid decline in behavioural habits and/or language and short survival and, despite our increased understanding of dementia-causing diseases, there are currently no effective treatments or cures for FTD on the market. With an ever-aging population, there is an urgent demand for reliable, unambiguous diagnostic methods and effective treatments for FTD to help alleviate these economic and societal pressures. Our research focuses on a multi-pronged approach to addressing this problem.

Targeting TAR DNA-binding protein 43 (TDP-43): TDP-43 is a ubiquitously-expressed protein in humans that binds to both DNA and RNA to perform a variety of functions. In healthy cells, it is primarily located in the nucleus and helps regulate RNA processing. In unhealthy neuronal and glial cells of large proportions of FTD patients, TDP-43 is often mislocalised to the cytosol and bundles into aggregates and stress granules, leading to loss of normal protein function and neurotoxicity.

Discovery of small-molecules that bind to TDP-43 with high affinity and specificity still eludes chemists. Developing compounds which do this will lead to the rational design of a variety of new therapeutics, ranging from new imaging agents (e.g. radiolabelled PET tracers) allowing for more accurate diagnosis of FTD, to inhibitors that ameliorate the adverse effects of this protein aggregation. This project will investigate structure-activity relationships of potential TDP-43 binders, starting from a 4-aminoquinoline-based lead compound which shows promising activity. **Supervisor:** Dr Jonathan Danon.

Inhibition of TDP-43 stress granules: TDP-43 which builds up in the cytosol (often after mislocalisation from the nucleus) tends to amass into aggregates and protective stress granules. It has been shown that inhibiting the formation of these stress granules can also reduce the number of TDP-43 aggregate inclusions in cells. The mechanism by which this occurs still needs further elucidation. However, no small molecules that can achieve this safely have been approved for treating FTD.

Work for this project will focus on the design, synthesis, and structural optimisation of several lead compounds that have been shown to reduce stress granule prevalence and decrease the levels of toxic, aggregated TDP-43 in cells. **Supervisor:** Dr Jonathan Danon.

Third generation PET tracers for probing microglial activation: Microglial activation is associated with immune response to neuronal injury and plays a key role in the initiation and progression of FTD. Microglia express the 18 kDa translocator protein (TSPO), which has consequently become a target for development of diagnostic imaging tracers for estimating microglial density. The widely-used first-generation PET tracer [^{11}C]PK-11195 exhibits high levels of non-specific binding and thus low signal-to-noise ratios (SNR), making it of limited use in detecting subtle fluctuations of TSPO expression. Second-generation ligands with improved SNR (e.g. lead compound [^{11}C]DPA-713) have been developed in recent years, but by and large suffer from undesirable binding affinity variation within the population due to a genetic variation in TSPO expression.

This project will continue work towards designing, synthesising, and testing ligands which overcome both of these hurdles, displaying high specificity and a "one-size-fits-all" binding affinity regardless of genetic polymorphism. This represents an enticing challenge in the search for effective third-generation TSPO PET tracers. **Supervisor:** Dr Jonathan Danon, **Co-supervisor:** Professor Michael Kassiou.

Please feel free to contact me to learn more about these and other projects available.

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My research group focuses on the design, synthesis and investigation of the properties of functional molecules. It spans a number of areas including (i) the synthesis and investigation of small molecule mimics of Nature's molecular receptors and enzymes (supramolecular chemistry); (ii) the development of new synthetic methods and (iii) application of these methods to the synthesis of both natural products and novel functional molecules. All projects involve synthesis, with some also involving physical and/or biological techniques. A number of collaborative projects are also available.

Anion receptors, sensors and transporters for environmental and biological applications: Anions play many roles in areas as diverse as biology, medicine, catalysis and the environment, so artificial anion receptors have numerous applications across all of these areas. However, the development of anion receptors that operate with high selectivity and affinity under physiological and environmental conditions is a significant challenge. In this project you will design and build receptors targeted to a range of anionic species such as sulfate and pyrophosphate and use these to detect anion concentrations or move anions across membranes. Projects are available in both developing the synthesis of these complex molecular scaffolds and in the evaluation of novel anion receptors, with the ultimate goal of producing receptors that can be applied to selectively detect or separate anionic species in the environment or in biological systems. These projects would suit students with an interest in either synthesis or techniques including the use of NMR, mass spec, UV-vis and fluorescence for the study of molecular interactions.
Supervisor (s): Kate Jolliffe

New responsive sensors for biological sensing: The field of fluorescent sensing has provided biological researchers with tools to visualise organelles, proteins, and chemical processes taking place within the cell. Projects in this area will involve designing fluorophores with improved chemical and biological properties, and preparation of responsive fluorescent sensors to understand the chemistry of the cell. These projects will suit with an interest in synthesis and photophysical studies (UV-vis, fluorescence), and could also include theoretical calculations and/or biological studies.
Supervisor (s): Kate Jolliffe and Liz New

Array-based sensing for biological studies: A key current challenge in biology and medicine is the measurement of chemical species within complex environments such as biological fluids. For example, subtle changes in enzyme expression can signal diseases such as cancer and arthritis. In this project, we will explore fluorescent sensing techniques for measuring disease markers, with the ultimate aim of clinical testing. In particular, we will utilise array-based technologies, which can concurrently screen multiple samples and analytes. This project will involve organic synthesis, photophysical studies, statistical analysis and testing of biological samples.
Supervisor (s): Kate Jolliffe and Liz New

Selective sensors for phospholipids: Living cells synthesise and metabolise over 1000 different lipids, which assemble to form bilayer membranes with lipid compositions that differ across cell types, sub-cellular compartments and even within a single membrane itself. However, the relevance of this vast structural diversity and the function of each different lipid is not yet understood. In order to provide information answering this important biological question, fluorescent probes that are selective towards different phospholipid headgroups are required. This project will involve the synthesis of novel sensors for phospholipid headgroups such as phosphatidylcholine and phosphatidylethanolamine. The selectivity of the sensors will be established in model membranes using fluorescence spectroscopy, then selective sensors will be evaluated in biological assays.
Supervisor (s): Kate Jolliffe

Please feel free to contact me to learn more about these and other projects available.

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The stilnox paradox – targeting ion-channels to treat neurological disease

The big problem: Stroke is the third largest killer and the leading cause of lasting disability, globally. According to the Stroke Foundation Australia, 65% of stroke sufferers are permanently disabled with 20% requiring institutionalisation.

The "Eureka" moment: http://www.abc.net.au/austory/i-am-sam-opener/8598606

'The Awakening' – Sam (severely disabled due to a series of strokes) was dosed with zolpidem (Stilnox) – a clinically approved sleeping pill. For the next hour, Sam was awake, speaking and functioning virtually normally.

The big question: How can a known sleeping pill, 'awaken the mind'? By modulating ion channels!

The next problem: Zolpidem is a hypnotic through its action on α1-γ2 binding sites and therefore has a gamut of negative side-effects (addiction, disillusion, sedation).

The project:

Aim – Discover novel scientific tool molecules and lead molecules for future development of selective α1-α1 modulators, that will be devoid of hypnotic effects occurring via α1-γ2 interaction.

Aim – Correlate in vitro pharmacology with in vivo efficacy using animal models of stroke and assess the pharmacokinetic parameters of promising lead candidates including zolpidem

Supervisor: Dr William Jorgensen (Possible dual supervision).

No pain, the aim – targeting ion-channels to treat neurological disease

The big problem: Neuropathic pain affects 1 in 5 Australians. Less than half of these patients obtain clinically relevant pain relief.

The "Eureka" moment:

Glycine receptors are inhibitory neurotransmitters and have well documented roles in neuropathic pain.

The big question: Why are there no glycine receptor modulators approved for the treatment of chronic pain?

The problem: It is difficult to rationally design molecules without either a 'scaffold' to build from (usually identified from a high throughput screen) or a crystal structure of the active binding site of the receptor.

The Solution: Amgen, last year published a crystal structure of the glycine receptor with an allosteric modulator bound to the receptor. Despite this, there has been little structure-activity-relationships performed around this scaffold.

The project:

Aim – Discover a library of CNS permeable compounds which act as potentiators of the GlyR

Aim – Discover GlyR potentiators of unique structures that are active in animal models of neuropathic pain.

Supervisor: Dr William Jorgensen (Possible dual supervision).

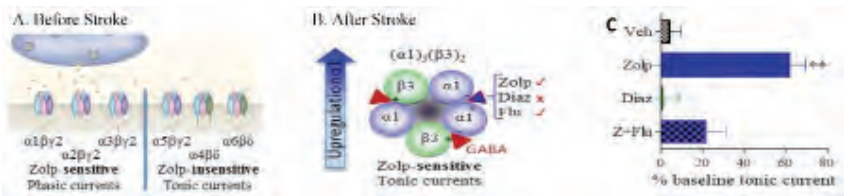

Fig 1: *A. Before stroke (normal brain), zolpidem modulates GABA by mainly activating synaptic α1βγ2 receptors (phasic currents) as they possess an α1-γ2 interface. Zolpidem is inactive at extrasynaptic $GABA_A$Rs (tonic currents) as they lack an interface where potentiation can occur. B. From 2-weeks after stroke, α subunits are upregulated, increasing α1-α1 interfaces. C. Zolpidem modulates GABA tonic currents at neurons via extrasynaptic $GABA_A$ receptors such as $(\alpha 1)_3(\beta 3)_2$ which possess an α1-α1 interface that only become present following stroke.*

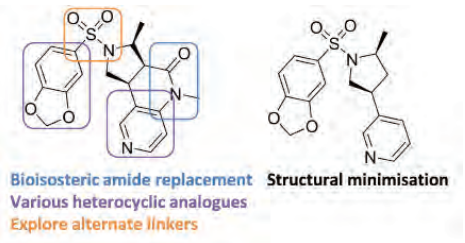

Fig 3: *Proposed modifications of AM-1488*

Please feel free to contact me to learn more about these projects at william.jorgensen@sydney.edu.au

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The field of medicinal chemistry is a key component in the drug discovery process. In the Kassiou group, we use synthetic organic chemistry to design and synthesise novel small molecules that target a range of diseases that affect the btain. The work in our laboratories has led to spin-off companies and first-inhuman trials of drug candidates. The projects below are only a sample of what we can offer, and projects can be tailored to suit the specific interests of any prospective students.

Treating Social Withdrawal

Conditions that commonly overlap with social withdrawal (SW) include depression, autism, addiction and social anxiety, among others. These might be considered as either the cause or the symptoms of SW. We are designing compounds that target the oxytocin receptor as a way of treating SW to target multiple disease states.

Oxytocin (OT) is a 9-amino acid cyclic peptide that exerts prosocial effects in mammals through activation of the OT receptor. However, as an oligopeptide it is a poor drug candidate and is not brain permeable. This project involves the synthesis of non-peptidic OT receptor agonists to elucidate how their chemical structure influences biological activity. **Supervisor:** Professor Michael Kassiou

Targeting Tau Protein Aggregation

One of the causes of disease progression in neurodegenerative disorders (e.g. Alzheimer's disease) is the malfunctioning and aggregation of tau protein. To date, research efforts involving single target approaches for treating tauopathies have not resulted in the discovery of any disease modifying therapies. However, multi-targeted strategies have shown promise and are being pursued at an increasing rate.

Currently we are developing compounds that modulate tau phosphorylation, promote tau clearance and inhibit tau aggregation. The long-term aim is to merge the pharmacophores of various combinations of these targets, to generate multi-target tau aggregation inhibitors. This project will continue work towards the synthesis of ligands to develop structure-activity relationships for the above targets. **Supervisor:** Professor Michael Kassiou.

Neuroinflammation

Immune cells in the brain can be activated in response to various events, including infection or traumatic brain injury, which in turn leads to neuroinflammation followed by neurodegeneration in several diseases. We develop small molecules that work against neuroinflammation as a treatment for these diseases. We also have a significant focus on imaging the neuroinflammation process by developing compounds for PET imaging. To achieve this we focus on two targets: Translocator protein (TSPO) and the purinergic $P2X_7$ receptor ($P2X_7R$).

First-generation PET tracers for TSPO exhibit high levels of non-specific binding and thus low signal-to-noise ratios (SNR), making them of limited use in detecting subtle fluctuations of TSPO expression. Second-generation ligands with improved SNR have been developed in recent years but suffer from undesirable binding affinity variation within the population due to a genetic variation in TSPO expression. This project will continue work towards synthesising ligands which overcome both hurdles, displaying high specificity and a "one-size-fits-all" binding affinity regardless of genetic polymorphism. **Supervisor:** Professor Michael Kassiou.

The $P2X_7R$ plays an essential role in inflammatory signalling as its activation leads to the formation and release of interleukin-1β, a proinflammatory cytokine which plays a major role in the inflammatory pathways underlying neurodegenerative processes. Our work involves developing ligands that bind to the $P2X_7R$ to inhibit its activation.

Supervisor: Professor Michael Kassiou.

Please feel free to contact me to learn more about these and other projects available.

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Our research projects are perfect for students who have a dual interest in both organic chemistry and biochemistry or molecular biology.

We take the molecules of life – proteins and peptides – and use chemical techniques to reprogram them for synthetic applications, ranging from catalysts for carbon fixation to molecular candidates for cancer therapy.

Our projects are very diverse, providing experience with a wide range of techniques: peptide chemistry, protein engineering, organic synthesis, DNA design, microscopy, and biophysics.

Engineered protein nanocages

We study *encapsulins*, naturally-occurring protein cages found in bacteria (Nat. Commun. 2018, 9, 1311). We aim to use encapsulins to create caged catalysts and therapeutics with novel biological properties.

1) Improving carbon fixation using caged Rubisco enzymes

In this project, you will prepare encapsulins filled with carbon fixation enzymes, and explore whether modifications to the amino acid sequence can help boost the reaction rate for carbon fixation.

The project will involve protein biochemistry, microscopy, and analytical chemistry.

2) Fluorescence studies on protein cages for drug delivery

In this project, you will prepare fluorescently-labelled encapsulins and use confocal microscopy to study their uptake behaviour in cells.

The project will involve molecular biology, spectroscopy and microscopy studies.

This is a joint project with Assoc. Prof. Elizabeth New.

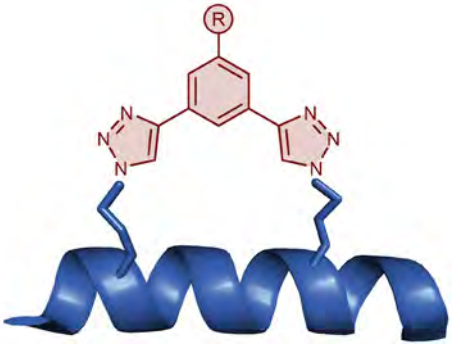
Targeting telomeres for cancer therapy

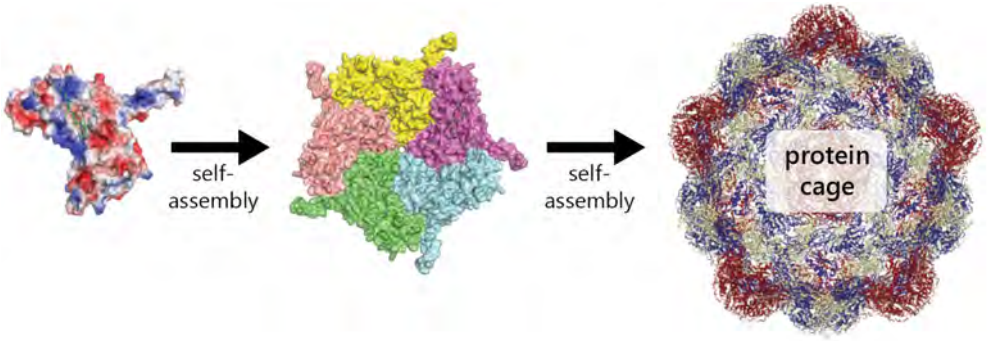
We synthesise *stapled peptides*, that are cyclised *via* their sidechains to improve stability and potency. Our peptides are designed to target a range of oncogenic protein targets that act at telomeres.

3) Inhibiting protein-protein interactions at telomeres involved in cancer

In this project, you will synthesise stapled peptides and fragment analogues to block telomeric proteins implicated in cancer, and conduct *in vitro* assays to determine their therapeutic potential.

The project will involve peptide and organic synthesis, biophysical analysis, and microscopy studies.





Please feel free to email Yu Heng to learn more about these and other projects available.

Also check out our group website: ***LauGroup.net***

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Biospectroscopy, medicinal inorganic chemistry, and molecular and cell biology will be used to understand the mode of action of existing drugs, the design of new drugs and to learn more about normal physiological and disease processes at a molecular and cellular level. Projects will centre on metal-based anti-cancer and anti-diabetic drugs, the active sites of heme proteins, or the use of biospectroscopy in disease diagnosis.

Spectroelectrochemistry of osmium ammine mixed valence ions: Mixed-valence complexes have played a central role in understanding electron transfer processes that are critical in biological electron transfer and materials research. Much of this understanding has arisen from studies on Ru(III/II) ammine mixed-valence ions with various bridging ligands, but Os anologues were much less accessible until general synthetic procedures were developed by Lay. The Os complexes are of particular interest because of strong intervalence electronic transitions in the near IR and IR regions of the spectrum where vibrational transitions normally dominate. This project will involve the synthesis of Os ammine complexes with bridging dinitrogen, N-heterocycle and organocyanide ligands and spectroelectrochemical experiments that include variable-temperature UV-Vis-NIR spectroelectrochemistry, Raman and IR spectroelectrochemistry, as well as a range of other spectroscopic techniques. The understanding of these basic spectroscopic properties leads the way towards advanced materials in which mixed valency is central to the functionality. **Supervisors:** Professor Peter Lay and Associate Professor Deanna D'Alessandro.

Biochemistry of Cr, Mo and V anti-diabetic drugs and supplements: We have amassed evidence to implicate potentially carcinogenic Cr(VI/V) complexes as the active forms of Cr dietary supplements that are widely consumed for fat reduction and the treatment and prevention of diabetes. We are using similar techniques to those used in the Cr studies to unravel the biochemistry of V and Mo supplements that are also anti-diabetics. The studies are aimed at producing safer and more efficacious treatments for the prevention and treatment of diabetes. These projects will include studies of the interactions of the complexes with biomolecules and cells using various spectroscopic techniques, including microprobes (X-ray, Raman, FTIR and fluorescence) and biochemical assays of protein expression, post-translational phosphorylation, sugar uptake and metabolism (glucose vs fructose), and protein-protein interactions. **Supervisor:** Professor Peter Lay.

Anti-cancer drugs: The anti-cancer properties of Ru complexes will be studied, since Ru complexes are one of few classes that have strong anti-metastatic activities. Investigations will involve studies on the ability of the Ru complexes to bind to blood proteins, extracellular matrices, the cell surface, and intracellular targets in order to bring about anti-metastatic versus cytotoxicity assays. Separate studies on one of Ga or V (with Dr. A. Levina) or Ru and/or Rh anti-cancer drugs including targeted drug delivery systems (with Prof. K. Jolliffe and A. Levina) will be considered. A project focused on any one of these metals could include a combination of synthetic organchemistry, biospectroscopy, and biochemical and cell biology assays. **Supervisors:** Professor Peter Lay and Professor Kate Jolliffe.

Imaging of organelles in cells: Changes in the biochemistry of specific organelles in cells are often one of the keys to understanding disease processes and, hence, to identify new drug targets and drug leads. Therefore, it is important to develop new imaging techniques to enable organelles to be identified in live cells and their biochemistry monitored. Specific fluorescence probes are useful for identification of specific organelles, but until recent developments in the New group, most of these are not useful for live cell imaging. We will combine developments in New group on novel organelle-specific fluorescent probes with 3D vibrational spectroscopic imaging techniques. These will be used to monitor organelle-specific changes in live cells during normal physiological processes (cell cycle), progression of disease and/or the effects of drug treatments. This research will be directed at either metabolic diseases or cancer. **Supervisors:** Professor Peter Lay and Associate Professor Liz New.

Vibrational spectroscopic studies for studies on disease processes and diagnosis: IR and Raman spectroscopic techniques can be used to diagnose various diseases and to understand disease progression at the biochemical level. The techniques rely on the ability of vibrational spectroscopic techniques to differentiate changes in amounts and distributions of biochemicals. Research could concentrate on cancer, malaria, neurodegenerative diseases or cardiovascular disease, in collaboration with colleagues in a number of hospitals and medical institutes. **Supervisor:** Peter Lay.

Please feel free to contact me to learn more about these and other projects available.

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Project 1: Development of high-affinity ACE2 mutants to combat COVID19

The human surface-expressed angiotension-converting enzyme 2 (ACE2) receptor has been identified as a functional receptor to mediate cell-entry of SARS-CoV-2–the etiological virus causing the current COVID-19 pandemic. SARS-CoV-2 infection has also been shown to lead to a substantial decrease in surface expression of ACE2 receptor, resulting in acute respiratory distress syndrome (ARDS)–one of the most devastating forms of acute lung failure.

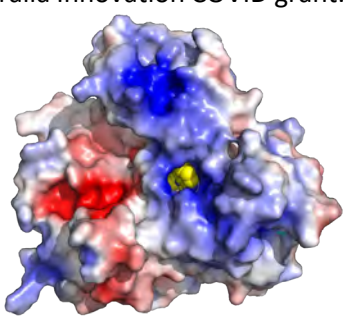
To address these ongoing issues, we aim to establish an expressed protein ligation platform to develop **high-affinity ACE2 mutants** which are capable of scavenging SARS-CoV-2 virus effectively in vivo whilst offering lung- and cardiovascular-protective effects.

The specific objectives include:

(1) Synthesising a library of high-affinity ACE2 peptide mutants.

(2) Synthesising full-length ACE2 proteins with distinct mutation pattern harnessing advanced protein ligation technology (***Nature Chemistry* 2017, *ACS Cent. Sci.* 2018**)

(3) Examining the binding affinity against SARS-COV-2 Spike protein using FACS, confocal microscopy and surface plasmon resonance technologies. Supervisor: Dr Xuyu Liu. Project funding by Therapeutic Australia Innovation COVID grant.

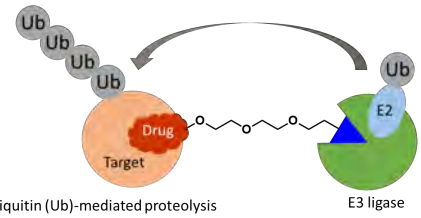


Project 2: PROTACs for cardiovascular disease

PROteolysis-TArgeting Chimeras (PROTACs) represent exciting new drug modalities. PROTACs are bifunctional molecules capable of binding simultaneously to a protein in the ubiquitinase complex as well as a protein target; this promotes selective proteolytic degradation of the target. This project aims to develop the first platelet PROTACs for the treatment of a range of thrombosis-related cardiovascular diseases, e.g. stroke. The project will involve synthesis of inhibitors of three key kinase targets (Pyk2, PI3K and Akt) and the conjugation of these to "degrader" units to assemble PROTAC libraries. The effectiveness of the novel PROTACs will be assessed in platelet aggregation and *in vitro* degradation assays. **This project will be co-supervised by**: Dr Xuyu Liu and Professor Richard Payne.

Project 3: Conditional knock-out of proteins in cardiovascular system by small-molecule modulators

Dissecting intricate protein signalling in cell requires precision control of the function and abundance of proteins on demand. Advanced genetic technology yields very limited information of dynamic cellular response to extracellular cues, i.e. cellular response to rapid oxidative stress in stroke. In contrast, chemical biology is making a huge translational impact to solve this contemporary challenge in dynamic physiology.



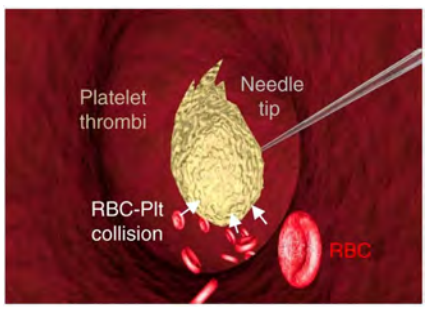
Ubiquitin (Ub)-mediated proteolysis E3 ligase

In this honours project, we will design and create a conditional knock-out system (**PROXY**) that leverages the potency of **PRO**TACs and **oxy**gen-sensing Arg/N-degron motifs, which will enable the investigation of transient protein functions in vascular tissues and platelets responding to intermittent oxidative stress. **This project will be co-supervised by**: Dr Xuyu Liu and Dr Mark White.

Project 4: Application of natural product-based probes to discover novel cardiovascular-protective targets

Despite the global burden of cardiovascular disease, the development of new cardiovascular drugs has stalled for over two decades. Recently, there is a considerable interest in the development of natural products extracted from healthy diets for cardiovascular-protective therapeutics. However, it remains a huge challenge to understand the molecular biology behind, which impedes pharmacological optimisation of these bioactive agents. In this honours project, we aim to apply cutting-edge chemical proteomics and chemical fluorescence technologies (***ACS Cent. Sci.* 2020, *Trends Biochem. Sci.* 2019**) to understand the intricate bio-activity of sulforaphane(SFN), a cardioprotective ingredient found in heart-healthy diets.

Please feel free to contact me to learn more about these and other projects available.



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A re-iterative approach to polycyclic ether construction: The marine ladder toxins, including the brevetoxins, ciguatoxins and protoceratins, are some of the most complex natural products that have ever been isolated. Indeed, maitotoxin is the largest non-proteinaceous molecules ever isolated from nature. Compounds of this class display spectacular and varied biological effects including anti-fungal, anti-cancer and anti-cystic fibrosis activity. In order to study the biological mechanisms of action of these compounds, an efficient and flexible synthetic strategy must be invented. The ambitious project for 2018 will involve the development of a contra-biomimetic re-iterative strategy for the construction of polycyclic ethers. **Supervisor:** Associate Professor Chris McErlean.

Total synthesis of canonical strigolactones: Everyone knows how plants grow, right? Wrong! Revolutionary discoveries in 2005 and 2008 mean that we are only just beginning to unravel the complex mechanisms under-pinning plant growth and development and a family of plant-signalling molecules called the strigolactones is the key to many of these processes. The McErlean group has developed an efficient strategy to access these critical molecules. The project for 2018 will involve the total synthesis of canonical strigolactones for use by international collaborators in the plant sciences. **Supervisor:** Associate Professor Chris McErlean.

Total synthesis of non-canonical strigolactones: Do molecules have to be large to be complex and difficult to synthesize? No! The non-cannonical strigolactones shown below are plant derived molecules whose functions are currently unknown. The unique combinations of reactive functional groups and congested stereochemical density, means that this family of compounds has never succumbed to enantioselective synthesis. All that is about to change. The project for 2018 will involve the total synthesis of non-canonical strigolactones for use by international collaborators in the plant sciences. **Supervisor:** Associate Professor Chris McErlean.

Point mutation using photoredox catalysis: Point mutations of polypeptides (such as proteins) traditionally involve altering a single base of DNA/RNA, and then use of a living cell to incorporate the new sequence into the ribosome for eventual production of a point mutant. Wouldn't it be faster, cheaper, and more direct to chemoselectively transform a single amino acid of a polypeptide into a vast array of natural and non-natural mutants? The McErlean group has recently developed a photoredox catalysed method for the generation of radicals in a chemoselective manner. The Jolliffe group are world leaders in the application of peptides scaffolds for selective ion sensing. The project for 2018 will involve the application of photoredox catalysed point mutation for the generation of therapeutic peptide libraries. **Supervisors:** Associate Professor Chris McErlean and Professor Kate Jolliffe.

Biodegradable and stimuli-responsive polymers for bio-applications: For application in bio-medical devices, polymers are required to be bio-compatible and degradable. Radical ring opening polymerisation (rROP) has emerged as a new tool to impart degradation profiles into synthetic polymers. Moreover, rROP will allow us to design inert biocompatible polymers that only activate specific properties (antibiotic, antifungal) upon triggered degradation. In this project you will employ rROP to introduce degradability into synthetic polymers using defined cyclic ketene acetals (CKAs). By carefully designing and synthesizing the CKA, not only will the required bio-properties be incorporated directly into the parent polymer, but the degradation products will also possess defined biological activities. In an increasingly environmentally aware world, this "whole-lifecycle" approach to polymer construction will represent a new direction in polymer science. Image: *Nature Chemistry* **7**, 771–784 (2015). **Supervisors**: Associate Professor Chris McErlean and Dr Markus Muellner.

Total synthesis of anti-infective peptide polyketide natural products: Recent advances in the discovery and characterization of biosynthetic gene clusters has revealed the existence of hybrid polyketide-peptide natural products that are produced through mixed non-ribosomal peptide synthesis (NRPS)-polyketide synthase (PKS) pathways. These fascinating metabolites have been shown to exhibit a plethora of biological activities, including potent activity against a range of disease causing pathogens and may therefore serve as novel lead molecules for drug discovery efforts. This honours project will involve the total chemical synthesis of the peptide-polyketide natural product janadolide, isolated from an Okeania sp. of marine cyanobacterium that has been shown to possess potent anti-parasitic activity. The project will involve a combination of modern solution- and solid-phase organic synthesis methods as well as biological screening. **Supervisors:** A/Prof Chris McErlean and Professor Richard Payne.

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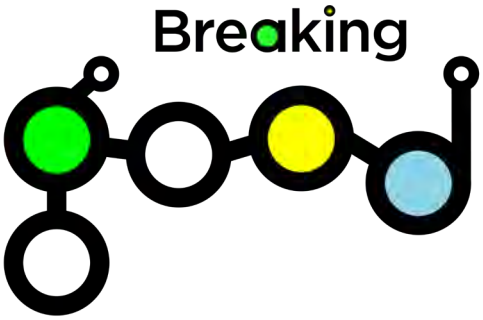
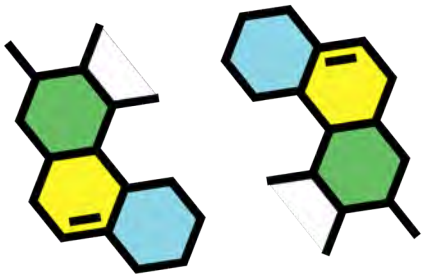
Research in the SCOPE (Science Communication, Outreach, Participation and Education) Group aims to connect people with science by making it more accessible. Using open science, education and outreach, our projects include open source drug discovery research for diseases such as malaria and mycetoma; research into public engagement with chemistry through science outreach and citizen science; and research into science education.

Open Source Drug Discovery: Solving wicked problems like antimicrobial resistance, malaria, or TB, requires new ways of thinking. Doing science 'open source' involves collaborating with *everybody*, sharing data and ideas in real time, using the tools and principles of open source software development. Join us to work on the Open Source Malaria or Open Source Mycetoma projects, and other projects in open source drug discovery.
Supervisors: A/Prof Alice Motion and Prof Peter Rutledge

Breaking Good – exploring citizen science projects in chemistry: Citizen science empowers members of the public to contribute to authentic research projects and knowledge creation. Breaking Good is a citizen science initiative that engages high school students, undergraduates and citizens to contribute to projects that improve human health. Join Breaking Good to develop process-style chemical synthesis for schools, to create and evaluate learning resources in chemistry or to explore ways to engage non-chemists in drug discovery projects.
Supervisors: A/Prof Alice Motion and Prof Peter Rutledge



Communicating chemistry: Chemistry is a tremendous force for good in our world, but not enough people know this. How do we spread the word? What are the most effective ways to communicate our subject to non-experts, to help people feel more connected to our discipline and to increase the general scientific literacy of our society?
Supervisors: A/Prof Alice Motion and Prof Peter Rutledge



Building a Modern Chemistry Kit: This project will seek to build a 'Hello Fresh' for chemistry experiments, where schoolteachers, lecturers or science outreach teams can order bespoke chemical demonstrations suitable for specific audiences or syllabus requirements. Investigations into the pedagogical importance of practical demonstrations in science education will inform your research into safe, suitable and effective demonstrations for diverse audiences.
Supervisor: A/Prof Alice Motion

Inclusive chemistry communication and education: This project will explore ways to make chemistry (and science more broadly) more inclusive in formal and/or informal settings. Science belongs to everyone, but some groups of people may not feel connected to, or represented in science, because of structural barriers that exist. In this project, you will research methods to improve the accessibility of science, and design and implement interventions to widen participation in science.
Supervisor: A/Prof Alice Motion

These are just some of many projects in the SCOPE Group Please feel free to contact me to learn more about these and other projects available.

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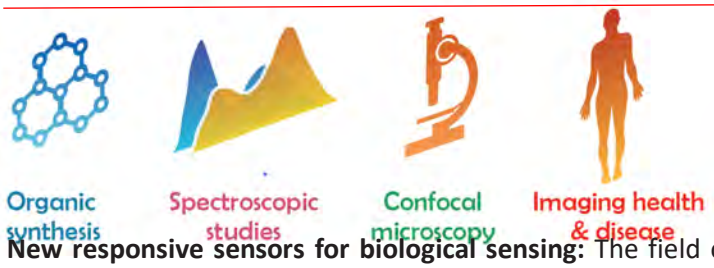
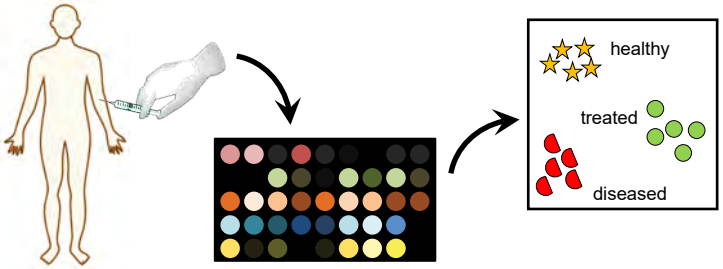
Our research involves developing fluorescent sensors that enable us to better understand medicine and the environment. Honours projects can include organic or inorganic synthesis, photophysical characterisation, spectroscopic studies and application of sensors in biological studies.

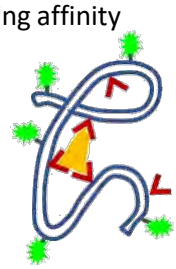


New responsive sensors for biological sensing: The field of fluorescent sensing has provided biological researchers with tools to visualise organelles, proteins, and chemical processes taking place within the cell. Projects in this area will involve designing fluorophores with improved chemical and biological properties, and preparation of responsive fluorescent sensors to understand the chemistry of the cell. These projects will suit with an interest in synthesis and photophysical studies (UV-vis, fluorescence), and could also include theoretical calculations and/or biological studies. *This is a joint project with Prof. Kate Jolliffe.*

Array-based sensing for biological studies: A key current challenge in biology and medicine is the measurement of chemical species within complex environments such as biological fluids. For example, subtle changes in enzyme expression can signal diseases such as cancer and arthritis. In this project, we will explore fluorescent sensing techniques for measuring disease markers, with the ultimate aim of clinical testing. In particular, we will utilise array-based technologies, which can concurrently screen multiple samples and analytes. This project will involve organic synthesis, photophysical studies, statistical analysis and testing of biological samples. *This is a joint project with Prof. Kate Jolliffe.*

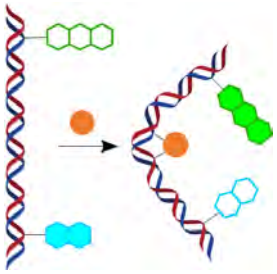


Functionalised polymers as fluorescent sensors: Polymers are an attractive scaffold for responsive sensors as they can be decorated with multiple binding/recognition sites, therefore increasing the selectivity and/or binding affinity for complex analytes. This project will involve the synthesis of responsive polymers functionalised with receptors and fluorophores that can be applied to environmental or biological studies. This project will involve polymer synthesis and photophysical studies. *This is a joint project with Dr Markus Muellner*



Fluorescence studies of synthetic organelles: Encapsulins are naturally-occurring bacterial compartments which are of interest for use as synthetic organelles and molecular cages for controlling chemical and enzymatic catalysis and for drug delivery In this project, you will prepare fluorescently-labelled encapsulins and use confocal microscopy to study their behaviour. The project will involve molecular biology, spectroscopy and microscopy studies. *This is a joint project with Dr Yu Heng Lau*

Using nanotechnology to build sensing molecules: DNA-based sensors offer many opportunities for sensing applications, including their ability to adopt many different 3D structures, to replicate biologically-relevant recognition events, the relative ease with which libraries of sensor candidates can be prepared and screened. This project will involve developing new DNA-based sensors for biologically relevant analytes, such as platinum-based drugs. The project can involve many different techniques, including DNA engineering, fluorescence spectroscopy, inorganic synthesis and biological studies. *This is a joint project with Dr Shelley Wickham.*



Single molecule spectroscopy of fluorophores: The ability to study the photophysical properties of compounds on the single molecule level has revolutionised science, from fundamental understanding to biological applications. The aim of this project is to design and synthesise new fluorophores that exhibit promising emission properties, and to carry out structure-property studies of their behaviour using a range of cutting-edge spectroscopic techniques. The project offers the opportunity for synthesis and spectroscopic studies, and will be of particular interest to students interested in the relationship between molecular structure and function. *This is a joint project with Dr Girish Lakhwani.*

Please feel free to contact me to learn more about these and other projects available.

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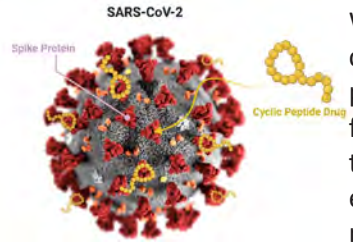
Organic Synthesis, Chemical Biology and Drug Discovery: Research in the group is focused on developing and utilising synthetic methods to solve problems in biology and medicine. We have used chemistry developed in our lab to generate drug candidates for a range of diseases.

Drug Discovery

Project 1:Novel Antiviral Development for COVID-19

The COVID-19 pandemic caused by infection with the novel coronavirus – SARS-CoV-2 – need little introduction. Within 9 months of the first reported COVID-19 case there have been 28 million cases and ca. 1 million deaths globally.

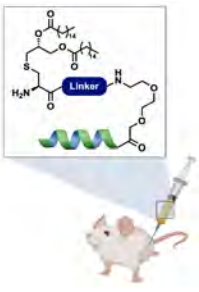


We have developed a cutting-edge peptide display platform to discover large families of cyclic peptides that inhibit viral proteins essential for cell entry and replication. In this Honours project you will synthesise a library of cyclic peptide antivirals using modified solid-phase peptide synthesis and assess their activity in biochemical assays. Compounds will also be screened against SARS-CoV-2 (with A/Prof Turville, Kirby Institute).

Supervisor: Prof. Rich Payne and Dr Toby Passioura.

Synthetic vaccines

Project 2: Glycopeptide cancer vaccines: In cancer cells there is a significant increase in the expression of a number of glycoproteins. This makes a cancer cell 'look' different to a normal cell and opens up avenues for the development of glycopeptide-based cancer vaccines. This project will use solid-phase peptide synthesis and organic synthesis to produce defined glycopeptides from cancer-associated cell-surface proteins. These will be covalently linked to immune-stimulating adjuvant molecules to elicit a favourable immune response. The compounds synthesised in this project will be used to generate tumour-selective antibodies in immunological studies thus allowing for their evaluation as anti-cancer vaccines.



Supervisor: Prof. Rich Payne and A/Prof Scott Byrne (CPC).

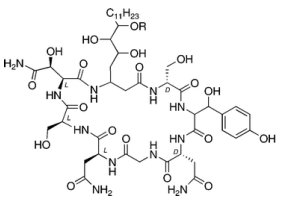
Total Synthesis

Project 3: Synthesis of therapeutic proteins *via* novel peptide ligation technologies:
Recently we have developed a number of new synthetic technologies that enable peptide fragments to be "stitched" together to generate therapeutic proteins (see *Nature Rev. Chem.* **2018**, 0122 and *Nature Prot*. **2019**, 2229). This project will involve the synthesis of modified variants of anti-coagulant and anti-inflammatory proteins produced by blood feeding organisms and their assessment in biological assays (see twitter.com/9NewsSyd/status/1265206053194600450).

Supervisor: Professor Rich Payne.

Project 4: Total synthesis of anti-infective natural products:

Recent advances in the discovery and characterization of biosynthetic gene clusters has revealed the existence of hybrid polyketide-peptide natural products which exhibit potent antibacterial and antifungal activities. This honours project will involve the total chemical synthesis of the antifungal peptide-polyketide natural product burkholdine (right) isolated from the bacterium *Burkholderia ambifaria*.



Supervisor: Prof. Rich Payne and A/Prof Chris McErlean.

Project 5: PROTACs for cardiovascular disease

PROteolysis-TArgeting Chimeras (PROTACs) are bifunctional molecules that bind simultaneously to a protein in the ubiquitinase complex as well as a protein target, thus promoting selective proteolytic degradation of the target. This project aims to develop the first platelet-specific PROTACs for the treatment of a range of thrombosis-related cardiovascular diseases, e.g. stroke and DVT. The project will involve synthesis of inhibitors of three key kinases (Pyk2, PI3K and Akt) and the conjugation of these to "degrader" units to assemble PROTAC libraries. The PROTACs will be assessed in platelet aggregation and *in vitro* degradation assays.

Supervisors: Professor Rich Payne and Dr Xuyu Liu

Please feel free to contact me to learn more about these and other honours projects available in the Payne Group: https://payneresearchgroup.com/

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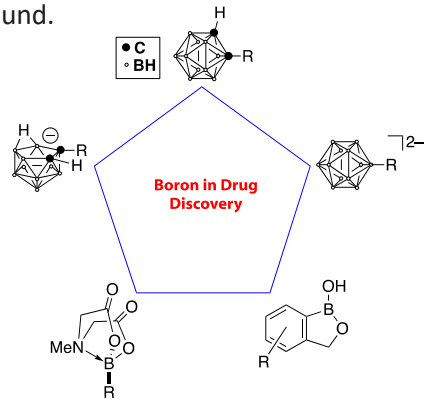
Our research group is a world leader in the synthesis of new molecules containing boron or gadolinium, with an emphasis on their applications in medicine. We are particularly interested in exploiting the unique properties of these two elements in cutting-edge cancer therapies. We are also interested in their incorporation into unique molecular scaffolds for binding to important biological receptors or as advanced materials. The Honours projects outlined below would ideally suit those students with an interest in synthetic chemistry and/or medicinal chemi

Gadolinium complexes as a new class of theranostic agents

The 5-year survival rate for patients afflicted with aggressive and intractable brain tumours (gliomas) is less than 4%. In this project, we will incorporate Gd^{3+} ions into tumour-selective agents in order to localize this metal near a critical sub-cellular organelle for application in binary therapies such as photon activation therapy (PAT) and neutron capture therapy (NCT). We have already demonstrated substantial and selective brain tumour cell destruction in the presence of a prototype Gd agent and synchrotron X-ray photons or thermal neutrons, the first time that either GdPAT or GdNCT experiments have been conducted in Australia. The use of Gd agents to target tumour cell mitochondria would open up new vistas in binary cancer therapies, with potential imaging applications in MRI.

Boron in drug discovery

Boron-based drugs are increasingly being investigated in many disease categories, with numerous pharmaceutical companies (e.g. Pfizer, GSK, and Takeda) dramatically expanding their boron research programs in recent years in the quest for novel drug candidates, e.g. Velcade® (bortezomib) which is used in the treatment of multiple myeloma. We are currently investigating the use of carboranes and other boron fragments as unique frameworks in new drugs for the diagnosis and treatment of aggressive and intractable cancers such as malignant gliomas. Biological studies may also be incorporated into the project, depending upon the student's own interests and background.



New tumour-selective chelators for multiple theranostic applications

We have recently designed a new class of organic chelators that can selectively target tumour cell mitochondria. These chelators can deliver high concentrations of metal ions to tumour cells with high selectivity over normal, healthy cells. There now exists the opportunity to exploit this family of chelators in a number of cutting-edge cancer therapies and also in tumour diagnosis (PET and MRI) involving a variety of medically-relevant metal ions (e.g. Gd^{3+}, Ga^{3+}, and Lu^{3+}).

Please note that no boron or lanthanoid chemistry background is assumed for any of these projects. These projects can be tailored to suit the specific interests of any student. Please feel free to contact me, check out the online Honours poster on Canvas, or visit our group website to learn more about these and other (jointly supervised) projects available.

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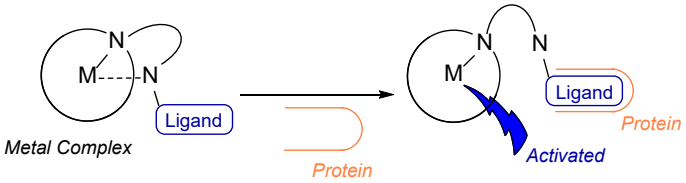
Research in the Rutledge group uses the tools of organic synthesis and chemical biology to develop new antibiotics, antifungals, and anticancer drugs, disrupt protein aggregation, and study protein function and evolution. We are also interested in chemistry education and communication research.

Antibiotics discovery: Bacterial resistance to antibiotics is an ever more urgent challenge for modern science and medicine. We are developing new ways to combat resistant bacteria, e.g.:

1. Building new organometallic antibacterials with high potency against tuberculosis and related species (with Prof Jamie Triccas, CPC).
2. Making 'resistance-activated' antibiotics.
3. Screening natural product extracts for new antimicrobial activity (with Dr Ern Lacey, MST).
4. Synthesising cyclobutanone β-lactams as β-lactamase inhibitors, using biocatalysis.
5. Mining microbial genomes for new bioactive compounds (with Prof Greg Challis, Monash).

Working on one of these projects you will develop skills in organic synthesis, chromatography and spectroscopy, or bioinformatics (genome mining project), and may have opportunity to conduct biological assays with our collaborators.
Supervisor: Prof Peter Rutledge

Evolving new old proteins: Ancestral sequence reconstruction is a technique that allows us to study protein evolution and resurrect ancient enzymes. We are using this and related approaches to investigate how oxygenase enzymes evolved over time and what they did before the world had oxygen, then apply this knowledge to build new, improved biocatalysts for the future.
Supervisors: Prof Peter Rutledge and A/Prof Nick Coleman (SOLES)



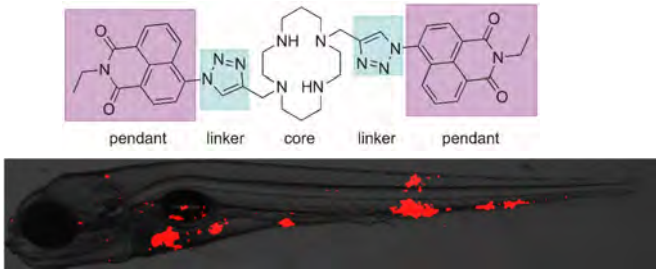
A 'target-activated metal complex'
Chem Eur J 2018 **24** 1573

Disrupting protein aggregation: amyloid fibrils are associated with protein mis-folding and disease (e.g. Alzheimer's and prion-associated diseases). But they also play key roles in structures that are vital to the survival and virulence of fungi. We have discovered a family of small molecules that disrupt the formation of amyloid fibrils. We are using these compounds to study amyloid assembly and develop new ways to treat diseases, both those that involve protein mis-folding, and those involving pathogenic fungi.
Supervisors: Prof Peter Rutledge and A/Prof Margie Sunde (SOMS)

Open Source Drug Discovery: Solving wicked problems like antimicrobial resistance, malaria, or TB, requires new ways of thinking. Doing science 'open source' involves collaborating with *everybody*, sharing data and ideas in real time, using the tools and principles of open source software development. Join us to work on the Open Source Malaria or Open Source Mycetoma projects, and other projects in open source drug discovery.
Supervisors: A/Prof Alice Motion and Prof Peter Rutledge

Communicating chemistry: Chemistry is a tremendous force for good in our world, but not enough people know this. How do we spread the word? What are the most effective ways to communicate our subject to non-experts, to help people feel more connected to our discipline and increase the general scientific literacy of our society?
Supervisors: A/Prof Alice Motion and Prof Peter Rutledge

Please feel free to contact me to learn more about these and other projects available.



Potent activity against mycobacterial infections like TB.
J Med Chem 2018 **61** 3595

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Oxygen (O_2) homeostasis is critical for mammalian life and is impaired in many human disorders. As a result, the molecular machinery responsible for coordinating O_2 adaptation have become prominent therapeutic targets. I have recently identified a novel O_2 sensing pathway (the Cys/Arg branch of the N-degron pathway), which could be manipulated to treat low O_2 (hypoxic) conditions such as cancer and cardiovascular disease. Using a range of techniques at the interface of chemistry and biology you will help characterise this system and develop chemical tools to investigate and manipulate hypoxic responses.

Chemical tools and probes

Project 1: Designing PROTACs for the conditional destabilization of proteins in cardiovascular systems

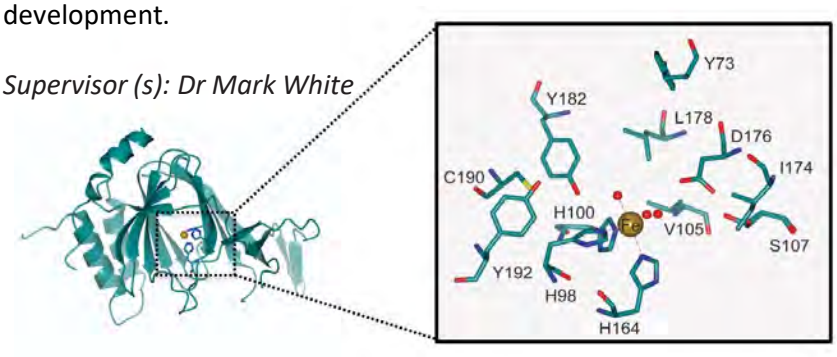
We will design and create a conditional knock-out system using small molecule conjugates that can regulate protein stability in response to oxidative stress by incorporating the O_2 sensing motif of the N-degron pathway into proteolysis targeting chimera (PROTAC) technology. This will enable the transient manipulation of protein function in cardiovascular tissue for therapeutic and diagnostic purposes.

Supervisor (s): Dr Mark White and Dr Xuyu Liu

Project 2: Identifying high affinity ligands of 2-aminoethanethiol dioxygenase

Using the high throughput screening platform mRNA display, we will identify, and subsequently optimise, novel high affinity ligands of the oxygen sensing enzyme 2-aminoethanethiol dioxygenase (ADO) so that its activity can be manipulated *in vitro* and *in vivo*. This will facilitate the discovery of new targets of the Cys/Arg branch of the N-degron pathway and provide a platform for drug development.

Supervisor (s): Dr Mark White



Biological chemistry

Project 1: Structural characterisation of a 2-aminoethanethiol dioxygenase complex

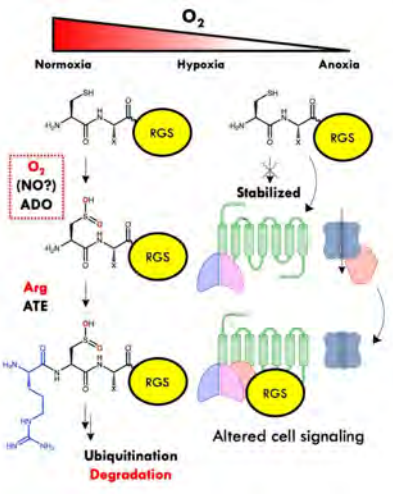
Using amber codon suppression, we will install unnatural amino acids into the substrate of the O_2 sensing enzyme 2-aminoethanethiol dioxygenase (ADO) so that a complex structure can be determined by X-ray crystallography. This will provide unprecedented information on enzyme chemistry and facilitate the rational development of chemical inhibitors to treat hypoxic disease.

Supervisor (s): Dr Mark White

Project 2: Dissecting the role and chemical contribution of nitric oxide in the N-degron pathway

Nitric oxide (NO) is reactive signalling molecule that controls a wide range of biological functions, largely through its interaction with metal centres and thiol groups. Through an undetermined mechanism, NO promotes protein degradation through the Cys/Arg branch of the N-degron pathway. Using synthetic substrates and a recombinant enzyme system, we will determine the role of NO, characterise its chemical intermediates and verify its biological function.

Please feel free to contact me to learn more about these and ot



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https://www.sydney.edu.au/nano/our-research/grand-challenges/nanorobotics-for-health.html

We use DNA as a molecular building block for self-assembling nanoscale structures and devices. With DNA we can make nanoscale tools – tweezers, spanners, wrenches and springs – and use them to understand cells and proteins. We use DNA nanostructures to develop new methods for in vitro diagnosis, and as templates for nanofabrication of electronic and plasmonic devices. We are also building sophisticated nanorobots to navigate complex environments and selectively deliver drugs in the body.

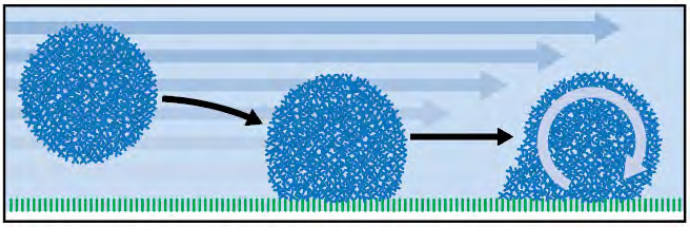
DNA-directed control of membrane signalling:
This project aims to design DNA-nanotechnology for processing optical signals in synthetic biological systems. We will duplicate the biological circuitry that transmits signals across lipid membranes. Ultimately, we aim to mimic the retina to develop a modular, lipid droplet-based system that can detect spatial patterns of light and convert them into chemical and electrical outputs for interacting with biochemical and cellular systems. This has potential future applications in brain-machine interfaces.
Supervisor (s): Dr Shelley Wickham

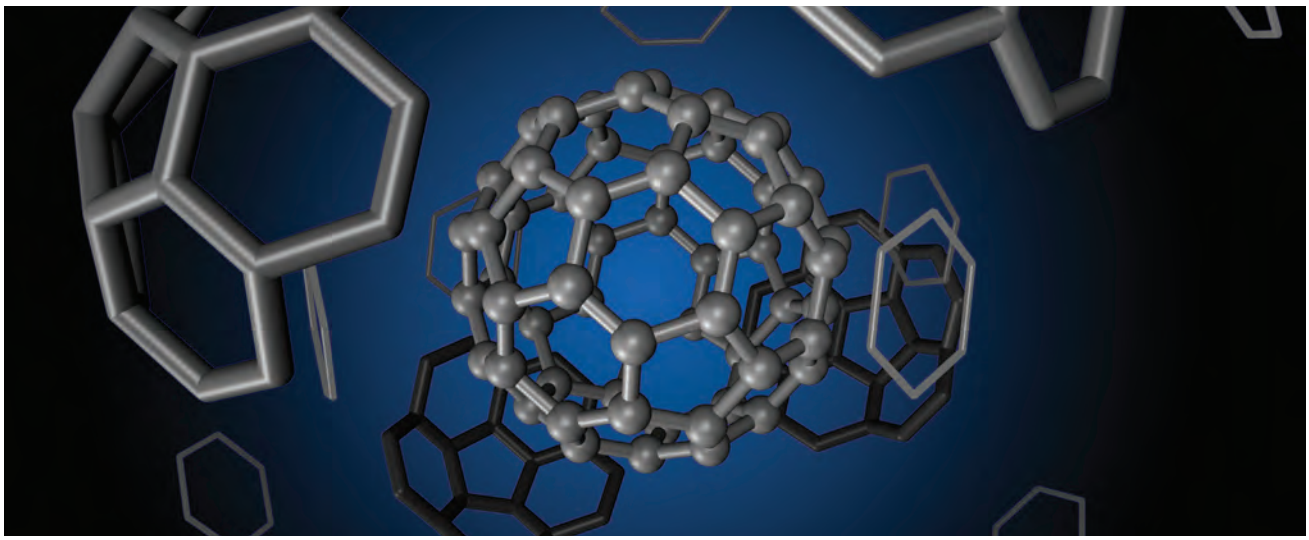
Navigating the brain along its spatial gradients using DNA nanorobots
Recent neuroscience breakthroughs have revealed spatial patterns in the brain's molecular structure, which represent a molecular 'postcode' of different brain areas. In this project, we will build a nanoscale machine that is able to navigate to specific locations in the brain using these patterns. We will design programmable molecular logic gates, which compare local chemical signals to stored values so that the nanorobot can determine its location in the brain. We will also build a 'brain-map-on-a-chip', which will serve as a controlled in vitro 'maze' in which to train and test these nanorobots experimentally. This work could ultimately lead to targeted drug delivery to specific parts of the brain.
Supervisor (s): Dr Shelley Wickham, Dr Ben Fulcher

Rolling nanobots on molecular obstacle courses:
Cells and viruses often move around by rolling on biological surfaces, a type of motility that is facilitated by weak interactions with surface-bound ligands. Building synthetic systems with this type of motility can teach us more about how biological systems work and can lead us to new bio-nanotechnological discoveries (eg. Nano Lett. 2019, 19(12), 9138). Using our expertise in DNA nanotechnology, surface functionalisation and microscopy this project will focus on building DNA-based nanobots that roll on surfaces patterned with tiny obstacle courses, allowing us to answer fundamental questions about biology with a view towards molecular medicines.
Supervisor(s): Dr Shelley Wickham, Jonathan Berengut

Nanotechnology to sense platinum in the blood
Platinum- based drugs are used in a large proportion of all chemotherapy regimens, but methods to measure drug levels in the blood are still lacking. This project will involve developing new DNA-based sensors for platinum in the blood.
Supervisor(s): Dr Shelley Wickham and A/Prof Liz New

Please feel free to contact me to learn more about these and other projects available.





COMPUTIONAL AND THEORETICAL; SOFT MATTER; AND MATERIALS CHEMISTRY

Research area:

Computational and theoretical, soft matter, materials chemistry

- Professor Peter Gill
- Professor Peter Harrowell
- Professor Stephen Hyde

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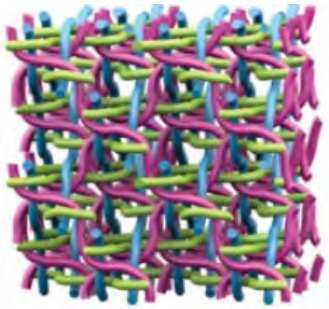
We are interested in using computer modelling and theory to understand the microscopic origins of fundamental aspects of crystallization, glass formation and the stability of novel solids.

While each of the projects listed involves computer modelling no previous experience in computing is required as instruction will be provided.

Woven Solids: The Birds Nest Problem

Woven textiles are remarkable – light, flexible, strong and, often, renewable. What new types of materials might we make if we could make three dimensional weaves? A bird's nest suggests one fascinating possibility – a rigid structure formed from stiff fibres without any bonding interactions. *In this project you will use computer simulations to study how stored bending energy in 3D weaves can produce rigid structures.* This study will contribute to fields as diverse as biology, architecture and material design. This project is a collaboration with Prof. Stephen Hyde.



Making Porous Metal Surfaces by Selective Dissolution

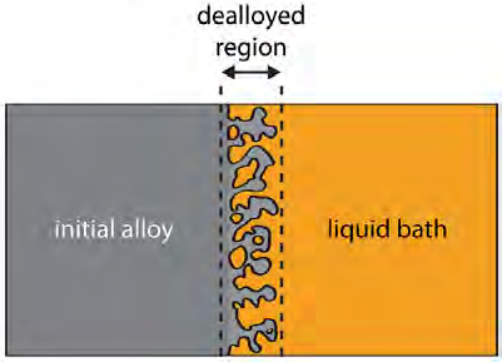
The efficiency of electrodes and catalytic surfaces are directly related to the surface area. Porous structures can increase this area by factors of 10^5. An exciting new strategy for generating these porous surfaces involves the use of selective dissolution of one metal species from a disordered alloy. *In this project you will use computer modelling to explore the process of selective dealloying and the stability of the porous structures formed.*

Machine Learning and Material Fabrication

The structure of a non-equilibrium solid like glass depends on its history. Vary the conditions of fabrication and you adjust the final material properties. We do not know how much variation is possible through control of the formation conditions. *In this project you will apply machine learning to identify the optimum fabrication methods for a modelled material to establish, for the first time, the limits on the properties that can be realistically achieved*. This project is a collaboration with Dr Stephen Whitelam at the Lawrence Livermore Lab, Berkeley, CA.

Thermal Scattering from Glassy Solids

The scattering pattern of x-rays and electrons from glasses resembles that of a liquid and so tells us little about the development of rigidity of the phase. Recent work in the group has established that another quantity, the amplitude of atomic motions, can provide a direct measure of developing solidity. *In this project you will use computer simulations to calculate the thermal scattering pattern and develop, for the first time, a method for extracting the Debye-Waller factor form experiments on glasses.* This project is a collaboration with the experimental group of Dr Amelia Liu at Monash University.



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I am interested in exploring the fundamental design principles of topologically complex structures of synthetic and biological materials, from folded RNA to biological and synthetic membranes. Key tools are non-Euclidean geometry, knot theory and low-dimensional topology.

Tangled molecular structures
Single-stranded RNA (pseudoknots)

RNA in many viruses adopts complex folds, often almost, but perhaps not quite, knotted. Are knotted structures likely to occur in natural and synthetic RNA strands? If not, how is that prevented? If so, what knots are likely? Some exposure to topology and/or knot theory would help in getting into this theoretical project.

Supervisor: Stephen Hyde

Membrane self-assembly
Folded vesicles & lamellar bodies

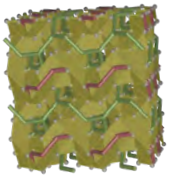
Nature has found very efficient ways to package a lot of membrane tightly, allowing transport of those packages and subsequent unfolding. "Lamellar bodies", for example, carry lung surfactants to their-lung surface at birth, allowing mammals to take their first breath (quickly!). This theory project will model relative (free) energies of possible shapes of (initially) spherical vesicles, to find 'optimal' shapes.

Supervisor: Stephen Hyde

Materials design
Woven Solids: The Bird's Nest Problem

Woven textiles are remarkable materials – light, flexible, strong .. and, in many cases renewable – that humans have relied on for over 10000 years. What new types of materials might we form if we could make *three dimensional* weaves? The project will examine how weave structures, fibre stiffness and friction contribute to the stability of the final material. Insights from this study will have application in fields as diverse as biology, architecture and material design. While previous experience in computer programming is useful, it is not necessary

Supervisors: Peter Harrowell, Stephen Hyde



DNA nanotechnology
Harnessing DNA to build 3D honeycombs

The base-pair recognition of DNA strands can be used to build synthetic structures at the molecular scale and up. In this project, we plan to use simple flat modules of DNA to assemble complex three-dimensional structures, in the spirit of an IKEA build, though a little smaller. The idea is to design DNA tiles with sticky edges, so under the right conditions tiles glue to each other to build three-dimensional honeycomb like constructions. The long-term goal is to make these constructions reversible, so they will build themselves, then disassemble, over and over. Though most suited to lab studies, a hybrid theory-experimental project, developing novel geometrical designs, is also possible.

Supervisors: Stephen Hyde, Shelley Wickham

Please feel free to contact me to learn more about these and other projects available.

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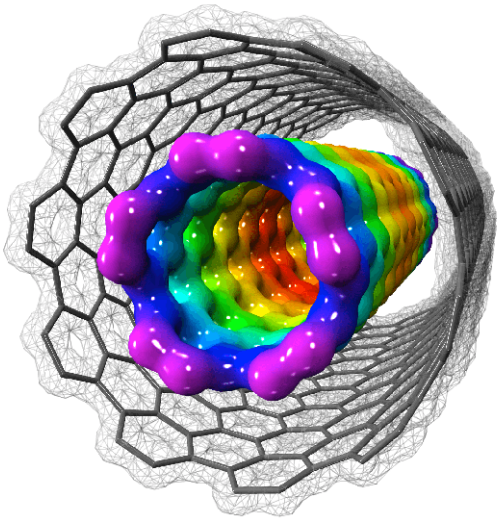
The University of Sydney Quantum Chemistry group is one of the hubs of the international "Q-Chem" collaboration (q-chem.com), which is developing new ways to use quantum mechanics to predict chemical behaviour. There are three phases to such developments:

Research Area 1

The Schrödinger equation describes the behaviour of electrons in a molecule but it is mathematically challenging to solve the equation for a large molecule in a reasonable amount of computer time. Our group therefore collaborates with leading groups in the world to **design new quantum chemistry algorithms** that find accurate approximate solutions to the Schrödinger equation for molecular systems. This arm of our research requires experience in calculus, linear algebra and related topics.



Research Area 2

Having found a good algorithm for solving the electronic Schrödinger equation, it is computationally challenging to implement the algorithm's equations as a useable program which runs well on a modern high-performance computer. Our group therefore collaborates with top computer scientists to **write cutting-edge software on cutting-edge hardware**, such as the Gadi supercomputer in Canberra or the Summit supercomputer at Oak Ridge. This arm of our research requires experience in programming.

Research Area 3

Having created high-performance (Q-Chem) software to solve the Schrödinger equation for the electrons in molecules, it is chemically challenging to apply that software to attack and solve chemical problems, by predicting molecular structure, bonding and reactivity "in silico", i.e. inside a computer. Our group therefore collaborates with experimental chemists, physicists and medical researchers, **using Q-Chem to perform simulations that complement and enrich laboratory experiments**.

Research projects are available in all three of these areas and a project is usually designed to fit the interests and expertise of the student. Our research is internationally recognized and the group leader, Prof Peter Gill, is currently the president of the World Association of Theoretical and Computational Chemists (watoc.net). For more information, contact Prof Gill.

CHEMISTRY EDUCATION

Research area:

Chemistry (education focused)

- Dr Stephen George-Williams
- Associate Professor Alice Motion
- Dr Reyne Pullen
- Professor Peter Rutledge
- Associate Professor Siggi Schmid
- Dr Shane Wilkinson

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In general, I am highly interested in how chemistry is taught (by us!) and learnt (by you!). Due to the sheer scope of activities that are involved in this process, I am constantly investigating a wide range of projects that span from the teaching laboratory, to the lecture/tutorial activities, to our assessment procedures, to the online space and even into virtual reality! I am always on the hunt for new and exciting ways to improve the teaching and learning of chemistry so please feel free to reach out if you have ideas beyond the projects outlined here.

Virtual reality for virtual learning: The discipline of chemistry requires a strong ability to link formal drawings and images (often referred to as 'symbols) to both the macroscopic level (i.e. what we see) and the microscopic level (i.e. the molecular and sub-molecular domain). Whilst we can discuss symbols and show macroscopic examples, it is incredibly difficult for us to truly explain microscopic interactions in a manner that ensures the student can 'see' what we, the teachers, see. By working with the X-reality hub within the School of Psychology, we can now consider how this could be best achieved using their state-of-the-art wireless virtual reality gear. With little literature precedent, this project represents a cutting-edge investigation into the utility of this exciting new technology in the learning space.

In this project, a student, in consultation with various academic members of staff, will choose from a variety of topic areas and generate the relevant virtual reality lessons themselves. The overarching research question, i.e. what effect the use of virtual reality has on student learning, will be investigated through the use of audio and video recorded trials, alongside concept inventories and practical tests. **Co-Supervisors:** A/Prof. Siegbert Schmid, Dr Reyne Pullen.

Rethinking undergraduate laboratories: The teaching laboratories in the school of chemistry represent one of the strongest learning opportunities for students. However, this can, at times, be undermined by experiments that do not engage students and have been noted to result in students completing the activity in 'auto-pilot' mode – i.e. they simply follow the steps with little to no critical thought with the only goal being the completion of the activity.

In this project, a student will aid in the design, testing and implementation of new laboratory activities within the school of chemistry. Evaluation of these activities will form the core of this research project through student trials, interviews and surveys. This will also require a strong consideration of the assessment procedures, encompassing pre-laboratory work, in-class observation and post-laboratory submissions. **Co-Supervisors:** A/Prof. Siegbert Schmid, Dr Reyne Pullen.

Measuring the ability of teaching staff to predict question difficulty: Previous literature has shown that students are often better at predicting the difficulty of exam questions as compared to academic members of staff. What is unknown however, is the direct factors that cause this variation and to what extent this difference is dependent on university or discipline area.

In this project, a student will obtain past exam papers and compare performance on individual questions against predictions made by academic staff. This will be compared against the demographics and research focus of the academic member of staff. If time permits, this project will expand to other schools within the university and potentially to other universities in Australia. Additionally, an intervention may be attempted wherein the academic member of staff may be supported in considering more literature-based means of determining question difficulty. **Co-Supervisors:** A/Prof. Siegbert Schmid, Dr Reyne Pullen.

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Teaching has always been one of my driving forces and chemistry education research allows me to better understand how I teach and how students learn. In contrast to disciplinary studies, working with people introduces a huge variety of factors that can be challenging to constrain and measure. The benefits of this is that there are always new and interesting questions to ask and explore. If you have ever taken an interest in teaching or would like to better understand the reasoning behind some of the educational experiences you might have had, I encourage you to get in touch!

Developing self-regulated learning strategies: A skill often taken for granted but essential throughout university and post-graduate life is the ability to regulate learning and place learned content within a broader context. Previous literature offers multiple approaches to developing this skill including the incorporation of prompting questions to guide students in developing these strategies.

This project will involve developing supporting materials to assist students with the development of self-regulated learning strategies based on literature recommendations. These materials will then be tested and measured through qualitative methodology to explore how students use these strategies. **Supervisor:** Dr Reyne Pullen.

Supporting the transition of secondary students to tertiary education: The transition from secondary to tertiary education can be a jarring move for many students. More so even, for those who may not have studied chemistry at all or for some time. Additionally, the first-year student cohort is often incredibly diverse with students from many academic and cultural backgrounds. As such, it is important to find the means to support their transition into first-year chemistry.

This project would aid in the design of an intervention to support students in a variety of possible ways. This might include addressing key assumed knowledge in first-year chemistry such as maths or facilitating the development of peer-learning groups. Finally, the success of these interventions will be measured using quantitative or qualitative methodologies depending on the sample size. **Supervisor:** Dr Reyne Pullen.

Measuring the effectiveness of embedding technology into learning activities: The needs of students are rapidly changing and alongside this the technologies available for education increase equally so. The question then arises, what technologies should be utilised? In what ways can these technologies support concepts or processes unique to chemistry? How do these technologies lead to a positive change – whether this is academic, cultural, or accessibility?

This project would involve developing an intervention based around the use of technology in some form (negotiated between myself and you) in the classroom. Depending on the technology we would measure its effect on one of the following: academic achievement, accessibility of abstract concepts, student time management or stress levels, and more. The scope of this project would begin within chemistry with potential applicability to other disciplines or other chemistry departments. **Supervisor:** Dr Reyne Pullen.

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My research interests are both in Chemistry Education and Functional Materials Chemistry. Chemistry Education research projects are designed to improve our understanding of how we best support student learning, in the widest possible sense. My group also focuses on developing novel and improved ceramic materials for use in a range of technological applications.

All projects on offer are student-centred, i.e. the direction these projects take will be based on your interests and strengths.

Inclusive Learning by Design

At the School of Chemistry, we aim to build an inclusive culture for staff and students. We have embraced changes in the undergraduate curriculum that offer diverse pathways for science students.

Projects in this domain will develop, for example, experimental procedures that allow students who are blind or low vision, to work in the laboratory independently and empower them to be active participants in their learning. Further projects can be designed with interested students.

Assessment Design

With increased emphasis on graduate qualities @Sydney and nationally, and moving from aspirational to verifiable, it is essential that we confirm that our assessments are fit for purpose or adapt them if they are not. We developed a framework to do this in straightforward fashion.

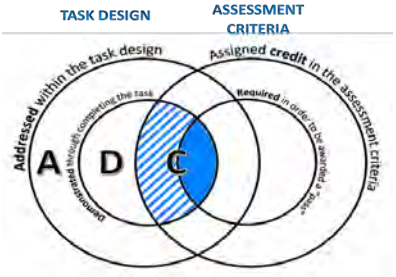


Figure 1. Two parts assessment: Is the targeted learning outcome covered in the assessment (you would hope so!), and is it weighted heavily enough in the marking scheme to confirm attainment of it? Applying this scheme will allow you to classify assessments and in doing so, important lessons can be learned for assessment design.

Supervisor: A/Prof. Siggi Schmid with other members of the Chemistry Education and Communication Research Theme

Sustainable energy storage

Rechargeable lithium ion batteries are widely used in portable electronics and hybrid or electric vehicles. Also, producing energy through sustainable means requires cheap and efficient storage to maximise the benefits. Compounds that can reversibly insert lithium have potential to be used in rechargeable lithium ion batteries. Our current program looks at a range of suitable compounds from defect perovskites to spinels and olivine type structures. This project aims to synthesise target compounds and to examine their chemical and electrochemical lithium intercalation behaviour. The products will be examined using X-ray and neutron diffraction at both national and overseas facilities.

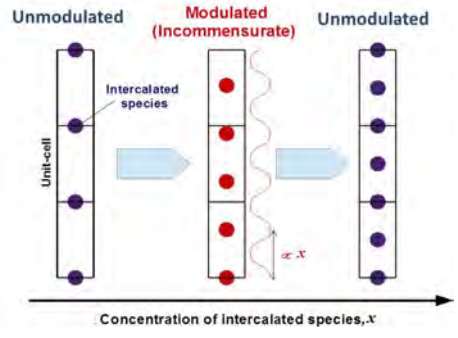
This project is in collaboration with Professor H. Ehrenberg, KIT, Germany and Dr William Brant, Uppsala University, Sweden.

Supervisor: A/Prof. Siggi Schmid.

Modulations and other Challenges

Electrode materials in rechargeable Li- or Na-ion batteries, that follow a solid-solution mechanism, change composition over very large ranges while maintaining their structure type. This is reminiscent of compositionally and displacively flexible systems that form incommensurate composite structures. While the compounds exist in 3D, their structure descriptions need higher dimensional space. Is that for you?

Figure 1. Schematic of electrode, with changing lithium concentration. Lithium ions are located where the modulation function (vertical centre) has its maxima.



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We live in a high-speed digital era where new technologies are merging all the time. My research focuses on exploring emerging technologies to empower educators with the latest tools that will shape students into the scientists of tomorrow. Additionally, these tools could be utilised to allow for more inclusive classrooms and laboratories by supporting students with diverse needs. Another aspect of a digital era is the generation of data, and lots of it. My research also looks at how we can effectively utilise this data to make evidence-based pedagogical decisions and predictions, improve the efficiency and quality of teaching, and deliver a personalised teaching experience to the students.

My projects span across the disciplines of chemistry, education, data science and programming with a particular interest in the use of augmented reality as tool in education.

Intelligence Augmentation (IA): In an Intelligence Augmentation (IA) system, artificial intelligence (AI) plays an assisting role in *enhancing* the human intelligence rather than replacing it. For example, AI would analyse data and present a series of options based on its algorithm and probability calculations but would not be responsible for *making* a decision. As humans, we could then *choose* which option to proceed with based on the AI proposed data as well as our own visual cues and "gut feeling".

We aim to develop an IA system for classrooms and laboratories that utilises Smart Glasses technology to stream AI-filtered data from student databases, learning management systems (eg CANVAS) and electronic laboratory notebooks (ELN) directly to the teacher. Acting on live data, a teacher would be able to adjust their classroom management by focussing their attention to flagged "at-risk" students during a classroom or laboratory tasks and address their needs. The system could also live-stream potential safety issues in a laboratory class so that the teacher can monitor or intervene before they become a problem.
Supervisor: Dr Shane Wilkinson

Augmented Reality in the Classroom: Augmented reality (AR) has been used in mobile apps for years from popular games such as Pokemon Go to applying filters on social media apps like Snapchat or Instagram. AR technology is a new tool we are looking to implement in the teaching and learning of science especially in the practical aspects of chemistry for both student and educator use. It has the potential to forge strong context-based learning through its ability to live-stream media and content to whatever the user is viewing and manipulating, in real-time. We aim to discover, develop and assess new AR applications that could be introduced in both undergraduate and postgraduate training and education.
Supervisors: Dr Shane Wilkinson, Dr Stephen George-Williams

"Bionic eyes": Smart glasses technology has the potential to promote an inclusive laboratory or classroom experience. The glasses can overlay, in real-time, alternate colours or contrasts to a colour-blind user so they can fully visualise all aspects of the content. In another example, smart glasses were used to convert vision to soundscapes (human echolocation) that allowed for near-to-completely blind users to gauge proximity, size and shape of objects. Another demonstrated example of smart glasses technology is their ability to translate live text and audio into different languages which would break down language barriers and open our classrooms to the world. We want to explore how these applications and technologies could be implemented and improved to allow for more inclusive laboratories and classrooms
Supervisors: Shane Wilkinson, A/Prof. Siggi Schmid, A/Prof. Alice Motion

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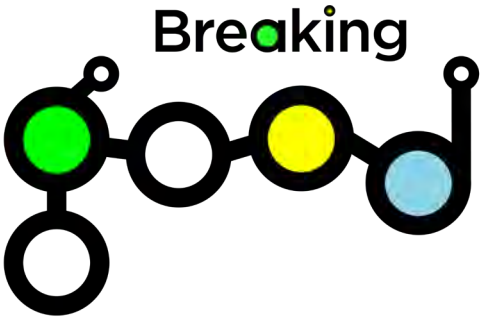
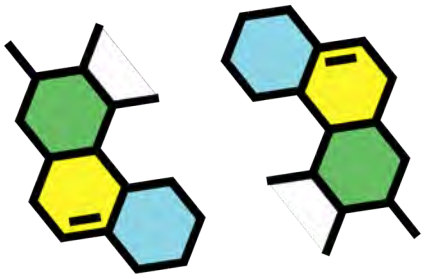
Research in the SCOPE (Science Communication, Outreach, Participation and Education) Group aims to connect people with science by making it more accessible. Using open science, education and outreach, our projects include open source drug discovery research for diseases such as malaria and mycetoma; research into public engagement with chemistry through science outreach and citizen science; and research into science education.

Open Source Drug Discovery: Solving wicked problems like antimicrobial resistance, malaria, or TB, requires new ways of thinking. Doing science 'open source' involves collaborating with *everybody*, sharing data and ideas in real time, using the tools and principles of open source software development. Join us to work on the Open Source Malaria or Open Source Mycetoma projects, and other projects in open source drug discovery.
Supervisors: A/Prof Alice Motion and Prof Peter Rutledge

Breaking Good – exploring citizen science projects in chemistry: Citizen science empowers members of the public to contribute to authentic research projects and knowledge creation. Breaking Good is a citizen science initiative that engages high school students, undergraduates and citizens to contribute to projects that improve human health. Join Breaking Good to develop process-style chemical synthesis for schools, to create and evaluate learning resources in chemistry or to explore ways to engage non-chemists in drug discovery projects.
Supervisors: A/Prof Alice Motion and Prof Peter Rutledge



Communicating chemistry: Chemistry is a tremendous force for good in our world, but not enough people know this. How do we spread the word? What are the most effective ways to communicate our subject to non-experts, to help people feel more connected to our discipline and to increase the general scientific literacy of our society?
Supervisors: A/Prof Alice Motion and Prof Peter Rutledge



Building a Modern Chemistry Kit: This project will seek to build a 'Hello Fresh' for chemistry experiments, where schoolteachers, lecturers or science outreach teams can order bespoke chemical demonstrations suitable for specific audiences or syllabus requirements. Investigations into the pedagogical importance of practical demonstrations in science education will inform your research into safe, suitable and effective demonstrations for diverse audiences.
Supervisor: A/Prof Alice Motion

Inclusive chemistry communication and education: This project will explore ways to make chemistry (and science more broadly) more inclusive in formal and/or informal settings. Science belongs to everyone, but some groups of people may not feel connected to, or represented in science, because of structural barriers that exist. In this project, you will research methods to improve the accessibility of science, and design and implement interventions to widen participation in science.
Supervisor: A/Prof Alice Motion

These are just some of many projects in the SCOPE Group Please feel free to contact me to learn more about these and other projects available.

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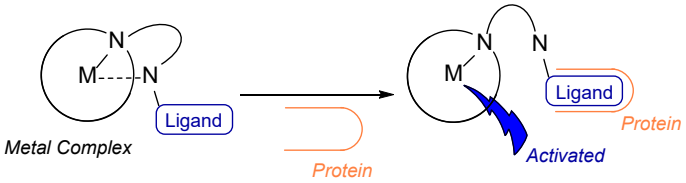
Research in the Rutledge group uses the tools of organic synthesis and chemical biology to develop new antibiotics, antifungals, and anticancer drugs, disrupt protein aggregation, and study protein function and evolution. We are also interested in chemistry education and communication research.

Antibiotics discovery: Bacterial resistance to antibiotics is an ever more urgent challenge for modern science and medicine. We are developing new ways to combat resistant bacteria, e.g.:

1. Building new organometallic antibacterials with high potency against tuberculosis and related species (with Prof Jamie Triccas, CPC).
2. Making 'resistance-activated' antibiotics.
3. Screening natural product extracts for new antimicrobial activity (with Dr Ern Lacey, MST).
4. Synthesising cyclobutanone β-lactams as β-lactamase inhibitors, using biocatalysis.
5. Mining microbial genomes for new bioactive compounds (with Prof Greg Challis, Monash).

Working on one of these projects you will develop skills in organic synthesis, chromatography and spectroscopy, or bioinformatics (genome mining project), and may have opportunity to conduct biological assays with our collaborators.
Supervisor: Prof Peter Rutledge

Evolving new old proteins: Ancestral sequence reconstruction is a technique that allows us to study protein evolution and resurrect ancient enzymes. We are using this and related approaches to investigate how oxygenase enzymes evolved over time and what they did before the world had oxygen, then apply this knowledge to build new, improved biocatalysts for the future.
Supervisors: Prof Peter Rutledge and A/Prof Nick Coleman (SOLES)



A 'target-activated metal complex'
Chem Eur J 2018 **24** 1573

Disrupting protein aggregation: amyloid fibrils are associated with protein mis-folding and disease (e.g. Alzheimer's and prion-associated diseases). But they also play key roles in structures that are vital to the survival and virulence of fungi. We have discovered a family of small molecules that disrupt the formation of amyloid fibrils. We are using these compounds to study amyloid assembly and develop new ways to treat diseases, both those that involve protein mis-folding, and those involving pathogenic fungi.
Supervisors: Prof Peter Rutledge and A/Prof Margie Sunde (SOMS)

Open Source Drug Discovery: Solving wicked problems like antimicrobial resistance, malaria, or TB, requires new ways of thinking. Doing science 'open source' involves collaborating with *everybody*, sharing data and ideas in real time, using the tools and principles of open source software development. Join us to work on the Open Source Malaria or Open Source Mycetoma projects, and other projects in open source drug discovery.
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Supervisors: A/Prof Alice Motion and Prof Peter Rutledge

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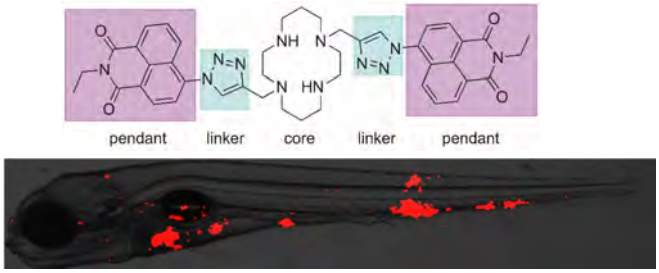

Potent activity against mycobacterial infections like TB.
J Med Chem 2018 **61** 3595