2020 HONOURS PROJECTS

School of Chemistry
USEFUL INFORMATION

Local and International students
Mid-year honours commencing in Semester 2, 2020 Applications close 30 June 2020

School of Chemistry application form can be found on the Honours in Science page

School of Chemistry
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

- 7 Dr Hamid Arandiyan
- 8 Associate Professor Deanna D’Alessandro
- 9 Associate Professor Meredith Jordan
- 10 Dr Ivan Kassal
- 11 Professor Brendan Kennedy
- 12 Professor Cameron Kepert
- 13 Professor Chris Ling
- 14 Professor Thomas Maschmeyer
- 15 Associate Professor Tony Masters
- 16 Professor Barbara Messerle
- 17 Associate Professor Siggi Schmid

### Self-assembled nanomaterials

- 19 Professor Phil Gale
- 20 Dr Toby Hudson
- 21 Dr Girish Lakhwani
- 22 Dr Markus Muellner
- 23 Associate Professor Chiara Neto
- 24 Dr Derrick Roberts
- 25 Professor Greg Warr
- 26 Dr Asaph Widmer-Cooper
- 29 Associate Professor Ron Clarke
- 30 Dr Jonathan Danon
- 31 Professor Kate Jolliffe
- 32 Dr William Jorgensen
- 33 Professor Michael Kassiou
- 34 Dr Amandeep Kaur
- 35 Dr Yu Heng Lau
- 36 Professor Peter Lay
- 37 Dr Xuyu Liu
- 38 Associate Professor Chris McErlean
- 39 Dr Alice Motion
- 40 Associate Professor Liz New
- 41 Professor Richard Payne
- 42 Professor Lou Rendina
- 43 Professor Peter Rutledge
- 44 Dr Mark White
- 45 Dr Shelley Wickham

### Molecular innovations in health

- 28 Dr Samuel Banister

### Computational and theoretical, soft matter, materials chemistry

- 47 Professor Peter Harrowell

### Chemical Education

- 49 Dr Stephen George-Williams
- 50 Dr Reyne Pullen
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
- Professor Barbara Messerle
- Associate Professor Siggi Schmid
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: CO₂ 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 CO₂ 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 CO₂ methanation, effectively activating the thermodynamically stable CO₂ 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 CO₂ 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 Communications 2015, 6, 8253; Energy Environ. Sci. 2016, 9 (1), 176-183). 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 electrolyzer 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 available.
Our research spans the areas of inorganic chemistry and materials science and focuses on the development of functional organic and inorganic materials that exhibit novel electronic and optical phenomena. Applications of our work range from the capture of greenhouse gases to address critical environmental challenges, to sensors, optoelectronics devices and photocatalysis for carbon dioxide conversion to fuels.

**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 based on mixed-valence metal clusters and redox-active ligands which exhibit stable radical states that can be generated using chemical, electrical or light as a stimulus. The opportunities for advances at a fundamental and applied level are immense, with potential applications ranging from new battery materials, to lightweight sensors, and new materials for energy-efficient gas separations. This project will also make initial steps towards the integration of conducting frameworks into solid-state devices, and the theoretical understanding of conduction in MOFs (with Dr Ivan Kassal). **Supervisor:** A/Prof. Deanna D’Alessandro.

**Photoswitchable 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 “photoswitchable molecular sieves” in which light can be used to modulate the size and electrostatic properties of the pores. This project will also make steps towards the integration of photoswitchable frameworks into membranes for industrial scale processes. **Supervisor:** A/Prof. Deanna D’Alessandro.

**Carbon dioxide capture and conversion:** The development of more efficient processes for carbon dioxide capture and conversion is considered key to the reduction of greenhouse gas emissions implicated in global warming. This project will involve the synthesis of highly porous MOFs and their integration into membranes for use in capture from major point sources including coal-fired power plants and natural gas wells. The goal of our research is to develop economically-viable materials that can capture and convert CO₂ in a concerted process to reduce emissions to the atmosphere and produce value-added products. **Supervisor:** A/Prof. Deanna D’Alessandro.

**Multifunctional electronic and magnetic materials:** The interplay between electron delocalisation and magnetism is ubiquitous in chemical and physical systems (e.g., solid-state superconductors, spintronics devices) and in metalloenzymes in nature; however experimental studies in which these phenomena coexist are extremely rare. This project will involve the development of metal complexes and MOFs with coexisting magnetic and electronic functionalities. **This project may be offered jointly with Profs Cameron Kepert or Peter Lay. Supervisor:** A/Prof. Deanna D’Alessandro.

Please feel free to contact me to learn more about these and other projects available.
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 of the observed H₂ can be accounted for by current atmospheric models. Given the increasing use of H₂ as a fuel, this is a significant shortcoming that needs to be urgently addressed. We have demonstrated a new photochemical source of H₂, 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 HO₂ radicals, two of the most important radicals in the atmosphere. We have postulated novel atmospheric reactions that may produce OH and HO₂.

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 stabilization of very internally “hot” atmospheric molecules, for example, after absorption of solar radiation, are completely 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 H₂ 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 H₂. These techniques are also applicable to other adsorbates, e.g. CO₂ and CH₄.

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.
We are developing cutting-edge theoretical tools—including quantum computing—to better understand fundamental chemical processes and to design superior devices, especially solar cells. A particular focus in our group are energy and charge transport, which underpin photosynthesis, solar cells, combustion, corrosion, batteries, and molecular electronics. Although the projects below range from pencil-and-paper theory to computer simulations, no computer programming experience is necessary.

### CHARGE AND ENERGY TRANSPORT

**Delocalised charge transport:** The transfer of charges (or excitation energy) from one molecule to another—perhaps the simplest chemical reaction—is a fundamentally quantum process. However, a fully quantum treatment of charge transport in most disordered materials—including most biological and chemical systems—can be computationally prohibitive. As a result, many models use purely classical concepts, such as molecule-to-molecule charge hopping, which can fail spectacularly, especially when the charges are delocalised over multiple molecules due to quantum effects. This project will develop fundamental new theories to treat the transport of delocalised charge with reasonable computational cost.

**Theory of organic electronics:** Organic semiconductors can be made into organic light emitting diodes (OLEDs) for displays and lighting, organic photovoltaics (OPVs) that promise truly green energy, and organic field-effect transistors (OFETs) for general-purpose flexible electronics. Despite their successes, many elementary processes in these materials are poorly understood. This project will develop new theories to describe charge and energy motion in organic electronics, especially OPVs, so that rational design can replace the current trial-and-error approach. A particular focus will be on relating device performance to the intrinsic molecular disorder. A project involving extensive device-level simulations or experiments is possible, co-supervised with Dr. Girish Lakhwani.

**Engineering quantum light harvesting:** Predictions that quantum coherence can dramatically affect light-harvesting efficiency have never been tested experimentally because no one has found a way to turn coherence on and off to see whether the efficiency changes. This project will design the simplest possible light-harvesting devices in which coherence-enhanced light harvesting can be demonstrated. In collaboration with experimentalists, the goal is to demonstrate the first instance of quantum control in an engineered light-harvesting complex.

### QUANTUM COMPUTERS FOR CHEMISTRY

**Simulating chemical reactions on quantum computers:** We are at the forefront of applying quantum computation to problems in chemistry, having shown that quantum computers could solve a wide range of chemical problems much faster than conventional computers. Today, chemistry is seen as a killer app for quantum computers, with chemical applications targeted by all the major quantum computing companies. This project is part of a large effort, with the group of Prof. Michael Biercuk in the School of Physics, to demonstrate the first simulation of a chemical reaction on a working quantum computer, in particular one based on trapped atomic ions. The questions we will be answering include: What is the best way to map a chemical reaction onto a quantum simulator? Can we exploit the motion of the trapped ions to mimic the motion of nuclei during a chemical reaction? What control protocols are needed to ensure a faithful simulation? This project can be co-supervised with Prof. Michael Biercuk, or undertaken by students pursuing a degree in physics.

We're a new group with lots of ideas, many not listed here. Drop us a line to see what else we're up to!
Our research focuses on the unique properties of transition metals that arise as a consequence of their partially filled d-shells. Many of these have unpaired electrons giving rise to magnetism and variable oxidation states. The projects all involve a mixture of synthesis, diffraction often centred on the use of major facilities (neutron and synchrotron) and computational/theory work. The balance depends on the project and the student.

**Energy, pyrochlores and perovskites:**
Energy security is one of the major challenges of the 21st century with both fuel cells and nuclear power being promoted. The binary oxide Gd₂Zr₂O₇ is currently of interest in both areas, being studied for use as an electrolyte solid oxide fuel cells which requires high ionic conductivity and as a host for immobilisation of radioactive waste which required no diffusion of cations. This project aims at understanding this apparent contradiction in properties. Our proposal is that anion disorder occurs independently of cation disorder and we are now keen to fully understand this process and to extend our observations to other pyrochlore type oxides such as Ln₂TiO₅. A third aspect of this work is to examine the structural stability of the key component of perovskite solar cells, the layered halide perovskites APbI₃. This project aims to establish the role the Pb²⁺ lone pair electrons play in their exceptional photovoltaic response.

**Structural and electronic properties of 4d and 5d oxides:** This project will build upon our discovery of an unexpected high magnetic phase transition temperature in Sr₂TcO₃ and Ca₂TcO₃. The work will explore the solid state chemistry of 4d and 5d metals isostructural with Tc(IV), especially Ru(V) and Os(V) to establish the role this has in the unusual magnetic properties of Sr₂TcO₃. We aim to prepare a number of double perovskites of the type A₂MLnO₆, M = Ru or Os, Ln = La or Y. We have developed world leading expertise in the analysis of L-edge X-ray absorption spectra of such oxides and a unique feature of this project will be to exploit this to understand the unique properties of these oxides. A second part of this project focuses on the importance of spin-orbit coupling in Ir containing oxides. This aims to build on the observation of unusual magnetostriiction in Ba₃BiIr₂O₉ and will explore both the role of spin-orbit coupling of the Ir cations and the potential for electron transfer between the Bi and Ir cation.

**What are the minerals on Saturn’s moon Titan?** In collaboration with Dr Helen Maynard-Casely, ANSTO: 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. With vast seas and lakes, sweeping dunes and dendritic channels, the evidence is mounting that the landscape of Titan has been shaped by both fluvial and pluvial processes. 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. Using the facilities at Sydney Uni and ANSTO this project seeks to understand exactly what the materials on Titan could be.

**Crystallographic studies of structural phase transitions:** This is my hobby, exploring the details of structural phase transitions and in particular understanding the coupling between orbital, magnetic and structural degrees of freedom. Whist the oxides find applications in magnetic devices this project focus on the fundamental crystallography. This project aims to prepare and structurally characterize Mn containing oxides of the type SrₓLnₓMnO₃ and will also explore the structures of the analogous Co containing materials.

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

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**Professor Brendan Kennedy**

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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. **Supervisor:** Professor Cameron Kepert.

Please feel free to contact me to learn more about these and other projects available.
The goal of our research is the discovery, characterisation and optimisation of 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, in order to guide the design and synthesis of improved materials. Honours projects almost always involve neutron and/or synchrotron X-ray scattering experiments, as well as complementary techniques such as electron microscopy and ab initio calculations of atomic structure, dynamics and electronic properties.

Surprising and (potentially) useful magnetism in lithium-ion battery materials: Despite the huge amount of research effort on lithium-ion battery materials, almost no work has been done on 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 and post-synthetic modification (e.g., ion-exchange), magnetic measurements, neutron diffraction, and building and testing batteries. **Supervisor:** Professor Chris Ling.

Stabilising the fastest of fast-ion conductors: Bismuth oxide is the best oxide ionic conductor known, but the relevant polymorph is only stable above 750°C. This can be fixed by “doping” with transition metals. However, the dopants also give rise to complex local oxide ordering, which degrades performance. This project seeks to understand how this works, and use the understanding to develop new materials. It will involve high-temperature synthesis, growing large (cm-scale) single crystals, neutron scattering and computational dynamics simulations. **Supervisor:** Professor Chris Ling.

**Novel hydrated oxides for mixed ionic-electronic conduction:** 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 to show MIEC, with FZF crystal-growth as a centrepiece. We will use the crystals for physical property and neutron scattering experiments, supported by ab initio energy and dynamics calculations. **Supervisor:** Professor Chris Ling.

Using high-pressure to shorten and strengthen metal-metal bonding: Negative thermal expansion (NTE), where volume expands on cooling, can arise through a range of mechanisms. Ba$_3$BiIr$_2$O$_9$, which we recently discovered, is a new case that works due to direct Ir–Ir bonding. The goal of this project is to synthesise new first-row transition metal oxides with analogous M–M bonding and magnetostructural effects. It will use high-pressure/high-temperature synthesis to stabilise these unusual structural forms, and low-temperature (down to 0.1 K) physical property and neutron scattering studies. **Supervisor:** Professor Chris Ling.

Structured polymer hybrids for better batteries and photovoltaics: Many functional properties depend critically on effective surface area. This project will use a new polymer-hybrid method to synthesise nanostructured materials for solid-state batteries and solar cells, with very high surface areas and efficient internal topologies. It will involve synthesis, characterisation on length scales from the atomic (X-ray and neutron diffraction) through the nano (electron microscopy) to the bulk (BET isotherms), and constructing batteries and solar cells to test under real working conditions. **Supervisors:** Professor Chris Ling and Dr Markus Muellner.

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

Cobalt catalysed conversions of renewable resources: The selective oxidation of hydrocarbons to alcohols, ketones and carboxylic acids is the largest industrial application of homogeneous (soluble) catalysts. The reaction is catalysed by cobalt complexes, frequently cobalt acetate derivatives. Although “cobalt acetate” was reported about 200 years ago, its structure is still incompletely understood – a variety of dimers, trimers, tetramers, octamers, etc., has been isolated from cobalt acetate and structurally characterised, however, they also interconvert in solution. This project examines the use of these catalysts in the selective conversion of renewable resources including lignocellulosic and algal biomass to value-added products such as specialty chemicals, high value monomers or pharmaceutical precursors. This project may be offered jointly with Prof Thomas Maschmeyer and Dr Alex Yuen. Supervisor: A/Prof Anthony Masters.

A functional model of the NiFe hydrogenase: Hydrogen is perhaps one of the earth’s oldest energy sources, providing the energy for some of the first microorganisms associated with the evolution of life. Today, the catalytic hydrogenations of fossil feedstocks, of nitrogen, and of commodity and fine chemicals (including asymmetric hydrogenations) are the highest volume industrial processes. In future, in addition to these chemical applications, hydrogen is again expected to provide energy for humankind on a large scale. Presently, the H₂/H⁺ interconversions and industrial hydrogenations are commonly catalysed by expensive metals, possibly unsuitable for large-scale (particularly distributed) use in the provision of energy. By contrast, the hydrogenase enzymes operate more efficiently using iron and nickel at their active sites. This project is targeted at the syntheses of functional models of bio-inspired catalysts, able to interconvert H₂ and protons. This project may be offered jointly with Prof Thomas Maschmeyer and Dr Alex Yuen. 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 only a few niche applications, although it can have a remarkably wide electro-chemical window. Stable, cheap, long life batteries and super-capacitors are the key to the roll-out of renewable energy technologies, such as those based on intermittent resources like solar and wind. 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 Thomas Maschmeyer and Dr Alex Yuen. Supervisor: A/Prof Anthony Masters.

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

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Work in the Messerle group is focused on designing organometallic catalysts that improve the reaction efficiency of organic transformations, thereby saving energy and decreasing waste produced during industrial chemical processes. Our multidisciplinary approach combines synthetic chemistry with surface science and nanotechnology. The work involves the development of novel transition metal complexes, as well as designing new catalysis methodologies using bifunctional catalysts targeting multistep reactions. The development of these catalysts stems from fundamental design concepts and encompasses both, mono- and multi-metallic complexes. The development of surface-bound (hybrid) transition metal allows us to access catalysts that are viable for industrial use, where recyclability makes them highly relevant to the design of greener chemical processes.

Multi-metallic catalysts for enhanced reactivity: Our pursuit of more efficient catalysts involves developing novel ligands that act as a scaffold around the transition metal (TM) to tailor the metal’s reactivity. One of our approaches for 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 the 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. Supervisors: Professor Barbara Messerle, Dr Indrek Pernik.

Bifunctional photo- and transition metal catalysts: When two different metals are used in the multi-metallic complexes, access to novel reactions can be gained, as each metal brings unique properties to the complex. Additionally, if one of these metals results in the formation of a photo-active species, the new bifunctional photocatalyst can be utilised in sequential reactions or in switchable reactions where reaction selectivity is controlled by applying either thermal or photochemical stimuli. Supervisors: Professor Barbara Messerle, Dr Indrek Pernik and Dr Sinead Keaveney (MQ).

New applications for surface bound (hybrid) rhodium and iridium catalysts: To develop industrially useful recyclable catalysts, we graft successful TM catalysts onto carbon surfaces to form hybrid catalysts. Once synthesized, the hybrid species are tested as catalysts for a variety of catalytic applications using organic substrates. Supervisors: Professor Barbara Messerle and Dr Max Roemer.

In addition to the projects described above, we are working on a variety of research topics such as the use of para-hydrogen and reduction of CO₂ gas.

Techniques: These projects include organic and organometallic syntheses using standard and air-free techniques under inert gas using gloves boxes and Schlenk lines. Compound characterisation and catalysis requires a broad suite of analytical techniques such as such as NMR- and IR-spectroscopy, mass spectrometry, X-ray single crystal diffraction and electrochemistry. The projects involving hybrid catalysts will additionally utilize surface characterisation methods like XPS and SEM/EDX.

Please feel free to contact Barbara to learn more about our projects and possible research opportunities. Please note that detailed knowledge of the involved chemistry and techniques is not required beforehand.
Research in my group focuses primarily on developing novel and improved ceramic materials for use in a range of technological applications. Chemistry Education research projects are designed to improve our understanding of how we best support student learning.

Sustainable energy storage: Rechargeable lithium ion batteries are widely used in portable electronics and start making an impact in hybrid and electric vehicles. In order to employ rechargeable battery technology in cars on a large scale battery performance, safety and lifetime need to be improved and research to that end is carried out on a massive scale. Furthermore, 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. We have a current program that looks at a range of suitable compounds from defect perovskites to spinels and olivine type structures. Two characteristics, the availability of interstitial or defect sites for the incorporation of lithium and the presence of redox active cations are essential for potential candidates. This project’s aim is to synthesise a number of target compounds and to examine their chemical reactions with lithium as well as their chemical and electrochemical lithium intercalation behaviour. The structures of all products will be examined using X-ray and neutron diffraction at both national and overseas facilities.

1. Rapid lithium insertion and location of mobile lithium in the defect perovskite Li_{2y}Sr_{1-y}Ti_{1-z}Nb_{2z}O_{3}. DOI: 10.1002/cphc.201200017
2. Designing a simple electrochemical cell for in-situ fundamental structural analysis. DOI: 10.1016/j.jpowsour.2013.03.086
3. Sodium uptake in cell construction and subsequent in operando electrode behaviour of Prussian blue analogues, Fe[Fe(CN)]_x(H_2O) and FeCo(CN)_y. DOI: 10.1039/C4CP02676D
4. In situ neutron powder diffraction using custom made lithium-ion batteries. DOI: 10.3791/52284
5. Co-ordination site disorder in spinel-type LiMnTiO_4. DOI: 10.1021/ic502747p

Colourful chemistry: Many colourful pigments that are still in use contain toxic heavy metals (e.g. PbCrO_4). The search for benign replacements has been successful for yellow pigments but not so much for the orange-red part of the spectrum. Metal nitrides and oxynitrides are often coloured and some already form the basis for new pigments. Synthesising and analysing a range of new mixed metal nitrides and oxynitrides from suitable oxides, this project endeavours to develop new coloured materials suitable as pigments in a range of everyday applications.

1. Modulated structures in the Ta_{2n}O_6-Al_{2n}O_6 system. DOI: 10.1071/CH12080
2. A (3+3)-dimensional "hypercubic" oxide-ionic conductor: Type II Bi_{4}O_{10}–Nb_{2}O_{5}. DOI: 10.1021/ja3109328
3. Structural investigation of tungsten bronze type relaxor ferroelectrics in the Ba_{x}Sr_{3-x}Ti_{4}Nb_{4}O_{15} system. DOI: 10.1017/S0885715614000980

Supervisor: Associate Professor Siggi Schmid.

Modulations and other challenges: Modulated structures constitute an intriguing class of materials that lack lattice periodicity (i.e. 3-D order) and yet are still perfectly long-range ordered. The full potential of these systems in terms of their applications remains to be explored. We have successfully investigated a number of systems over recent years involving lead-free piezoelectric ceramics as well as a family of transition metal borates with non-linear optical properties. The proposed projects encompass a wide range of both synthetic chemistry and characterisation techniques, in particular X-ray and neutron powder and single-crystal diffraction as well as electron microscopy using in-house equipment as well as instrumentation at major national and overseas research facilities.

1. Modulated structures in the Ta_{2n}O_6-Al_{2n}O_6 system. DOI: 10.1071/CH12080
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Supervisor: Associate Professor Siggi Schmid.

Please feel free to contact me to learn more about these and other projects available.
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
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, 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 organelle. **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 markers 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.

**Chemical uncouplers based on fatty acid flip-flop:** Uncoupling proteins present in the mitochondria inner membrane dissipate the energy of oxidative phosphorylation into heat bypassing ATP synthesis. They are important in the regulation of mitochondria membrane potential, fatty acid metabolism and the level of reactive oxygen species (ROS). Small molecule anion receptors can mimic their function by assisting the flip-flop of fatty acid anions across lipid bilayers allowing protons to permeate through the membrane. This project aims to develop highly carboxylate-selective anion receptors that can perform the fatty acid-dependent uncoupling function without the side effect of facilitating chloride transport. You will synthesise anion receptors and study their anion binding affinity and membrane transport selectivity. Compounds with desired transport properties will be sent to collaborators for mitochondrial uncoupling studies, to further explore potential application as anti-obesity or anti-aging drugs. **Supervisor:** Professor Philip Gale.

Please feel free to contact me to learn more about these and other projects available.
Predicting and designing the structures made by the self-assembly of particles is a key requirement for a new generation of advanced materials. Many fundamental questions are still open. The group’s research involves the computer simulation of complex materials, concentrating on issues of structure and dynamics. All of the projects are done with computational experiments, but all can be done without previous experience of programming.

What is it about the shape of a particle that determines how it packs?
One of the big challenges in crystal engineering is to predict how nanoparticles will self-assemble into crystalline arrays. Some particle shapes fill space better than others, but when they self-assemble, they all try to do the best they can. We have found that individual particle properties like symmetries, concavity, and aspect ratio all play a role in how dense they can collectively be arranged. But so far we cannot explain why some shapes pack in an unusual complex pattern whereas others are quite simple. Some chiral molecules crystallise as pure enantiomers while others prefer to form racemic crystals. Why? Some achiral molecules become chiral during crystallisation. Why? Supervisor: Dr Toby Hudson.

Protein structure prediction - unfolding knots with extra dimensions: The native state of a protein almost never includes a knot. But computational structure prediction is often plagued by knots and other tangles that are slow to resolve, and thus dramatically reduce the effectiveness of the search for a prediction. We have previously found that for network materials with similar frustrating tangles, the introduction of additional compact spatial dimensions allows these frustrations to easily unfold, while still allowing us to easily draw the structure back to a realistic three-dimensional structure. This project would apply this promising methodology to the important field of protein structure prediction. Supervisor: Dr Toby Hudson.

Building billion year old glass in a day: Recent experiments using physical vapour deposition of a warm thin film show that the free surface allows molecules the flexibility to search around a bit before they get stuck. This creates a material which is extremely stable compared to normal bulk glasses, and is equivalent in most respects to a glass which by some estimates has been aged for billions of years. In this project, you will simulate this process and the materials it creates. Supervisor: Dr Toby Hudson.

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 the theoretical understanding of these systems is still in its infancy – there is even still wide disagreement on how to define a random packing. Everyone is clear that they are not crystalline, but if you shake them just right, they can become more ordered. This project will investigate the ways in which random packings of a series of different particles are related to the ideal crystal structures of those same particles. Supervisor: Dr Toby Hudson.

Porous nanoparticle superlattices: Nanoparticles can now be made with exquisite control of shape and are becoming increasingly important as building blocks for new high-tech materials. Mixtures of particles with directional interactions are attractive candidates for making a new family of porous superlattices, which have applications in catalysis, sensing, and optics. You will explore the range of superlattices that can be made, using Monte Carlo simulations and by extending a structural search algorithm. Interesting structures may be synthesized by collaborators in Japan or the USA. This is a joint project. Supervisors: Dr Toby Hudson and Dr Asaph Widmer-Cooper.

Structure and stability of molecular crystals: The stability and structure of molecular crystals is of great interest in pharmacology and the development of functional thin films. In one project, you would calculate the thermal expansion of molecular crystals – an experimentally accessible property that provides a window into the trade off between optimal packing and optimal vibrational freedom, a trade off that is particularly sensitive to molecular shape. This is a joint project. Supervisors: Dr Toby Hudson and Professor Peter Harrowell.

Please feel free to contact me to learn more about these and other projects available.
MOLECULAR PHOTOPHYSICS RESEARCH GROUP

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 the optoelectronic properties of novel nanoscale semiconductor materials for solar energy harvesting, polarisation switching and polariton lasing. Our research underpins various research projects within the ACEX and beyond.

Probing energy transfer one molecule at a time: Our group is heavily invested in understanding molecular parameters that underpin the excitonic behaviour at a nanoscale. An exciton is a Coulombically bound electron-hole pair that is generated in a material either by light absorption or electrical charge injection. As the size of devices decreases, single molecules dominate optical processes such as energy transfer. In our group, we use single molecule spectroscopy to study optical processes occurring at a single molecule level otherwise obscured while using conventional spectroscopic methods that ensemble averages molecular heterogeneity. For example, single molecules show fluorescence blinking, which causes random switching of emission between on and off states. In this project, we will investigate blinking dynamics in low dimensional systems and identify its origin. **Supervisor:** Dr Girish Lakhwani.

Faraday rotation in organic semiconductors: Society’s over-reliance on information exchange around the world hinges critically on ultrafast data communication using light signals. Modern optical data communication works at high bit rates and therefore polarization switches have to be very fast (< 1ns). Understanding dynamics of polarization decay and dispersive transport of excitons as a function of device morphology is critical in underpinning material parameters required developing ultrafast polarization switches. This project will use a range of complementary experimental approaches to study polarization switching and Faraday rotation in an emerging class of organic semiconductors. **Supervisor:** Dr Girish Lakhwani.

Chiroptical phenomena in conjugated systems: π-conjugated materials (CMs) have proven to be cheap, easily processable and flexible alternatives to silicon for applications in thin film solar cells and light emitting diodes. However, the optical and electronic properties of CMs depend strongly on the polymer organisation within a nano-aggregate that isn’t well understood. In our lab we use Circular Dichroism (CD) spectroscopy to study molecular organisation of chiral materials by measuring difference in absorbance of left- and right- circularly polarised light in ground and excited states. In this project you will experimentally study structure-property relationships of chiral analogues of CMs using CD spectroscopy and characterise their organisation in nano-aggregates. **Supervisor:** Dr Girish Lakhwani.

Time resolved spectroscopy: Soft condensed matter covers a broad range of fields from biology to optoelectronics and photonics. Within this, conjugated materials demonstrate both ordered and disordered phases depending on the chromophore arrangement. While strong electronic coupling between chromophores promotes delocalization of the optical excitation, weak coupling makes energy vary from site to site controlling the energy and charge transfer central to the operation of optoelectronic devices. This project will use time-resolved spectroscopy to identify role of disorder on energy transfer. **Supervisor:** Dr Girish Lakhwani.

Device physics of organic solar cells: Photo-generated free charges in organic solar cells must be transported to the respective electrodes before they can recombine resulting in loss of current. Recently, several research groups have demonstrated that by modulating singlet and triplet charge transfer states, charge recombination can be reduced significantly. In this project, you will fabricate devices and identity strategies to reduce charge recombination thereby providing design rules for highly efficient solar cells. **Supervisor:** Dr Girish Lakhwani.

Please feel free to contact me to learn more about these and other projects available.
A multidisciplinary research effort is focussed on finding new ways to tackle current issues in the fields of sustainable materials, renewable energy and the diagnosis and treatment of diseases. The ability to control the synthesis of materials at the nanoscale allows us to produce tailor-made nanomaterials with distinct properties. In our group, we are interested in finding intuitive and new ways to access unprecedented polymeric and hybrid nanostructures. Our aim is to produce complex and multifunctional nanoscale materials for applications in catalysis, batteries and nanomedicine. Polymer science provides the ideal playground for creative materials design. In addition, the Australian Centre for Microanalysis and Microscopy and the Charles Perkin Centre provide a generous pool of microscopes and cell culture facilities allowing us to investigate our materials with state-of-the-art instrumentation. You can find more information on polymer architectures and their emerging applications by browsing through our publications at www.polymernanostructures.com.

Our group is very interdisciplinary and polymer science in general connects many chemistry areas. In addition, polymers find use as materials, and can therefore also feed into engineering and pharma disciplines. We honour the diverse interest 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.

**Shaping nanomedicines:** 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 shaped particles. In this project, we will build on our findings and develop a new nanoparticle platform to study the efficacy and usefulness of cylindrically shaped and ring-shaped polymers in biomedical applications and tumour penetration. **Supervisor:** Dr Markus Muellner.

**Virus mimics:** 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 Muellner.

**Mesostructured materials:** 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 Muellner and Prof. Chris Ling.

**Nanohybrids:** Cylindrical polymer brushes are unimolecular templates that can be used to produce one-dimensional hybrid nanomaterials, such as nanowires and nanotubes. We have developed strategies to produce organic/inorganic hybrid nanomaterials suitable for applications in catalysis or photovoltaic devices. In this project, we will progress this work and develop polymeric architectures (including some that are based on cellulose nanocrystals) that act as nanoreactors to produce novel hybrid nanomaterials. This multidisciplinary research aim merges the fields of chemistry and materials science. **Supervisor:** Dr Markus Muellner.

**Protein corona:** Proteins are known to stick to surfaces. This does not exclude nanoparticles. But by controlling the adsorption of specific proteins, the identity and hence properties of nanoparticles can be altered in a way so that the surface properties enhance cellular interaction by active targeting. In this project we seek to understand this phenomenon better through proteomics and cell culture studies. **Supervisor:** Dr Markus Muellner.

Please feel free to contact me to learn more about these and other projects available.
Our area of research is physical chemistry of interfaces, a multi-disciplinary field spanning the disciplines of chemistry, physics, nanoscience and materials engineering. In particular 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. We are interested both in understanding fundamental mechanisms and in their application in nanotechnology. Research projects are available in the following areas.

**Patterned coating for water capture:** This project addresses the study of micro-patterned polymer surfaces that collect water from the atmosphere, as part of a large multidisciplinary Grand Challenge project involving academics from across the University. The surfaces are patterned, consisting of isolated hydrophilic droplets on a hydrophobic background. The produced patterns mimic the surface structure that is present on a beetle native of the Namib desert, which collects drinking water on its micro-structured back. We are using technology that will help us collect water without any energy input, in a delocalised fashion. Future research could lead to the use of these coatings in the real-world, to provide decentralised and convenient water collection means to alleviate water scarcity. For a video illustrating the principle visit [https://www.abc.net.au/catalyst/lotus-effect/11013104](https://www.abc.net.au/catalyst/lotus-effect/11013104).

**Supervisor:** Associate Professor Chiara Neto.

**Slippery liquid-infused surfaces:** Liquid repellence is important in 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. We will work on two new approaches for the fabrication of such liquid-like surfaces: the first is a nano- and micro-structured polymer surface that is infused with a compatible lubricant (expanding on our discovery of slippery polymer wrinkles); the second is a liquid-like thin polymer layer that is grafted to a solid substrate (in collaboration with Dr Markus Muellner).

**Supervisor:** Associate Professor Chiara Neto.

**Measuring slip in microfluidic devices:** Overcoming the huge hydrodynamic resistance that slows down liquid flow in confined spaces is a technical and scientific challenge. This project will explore the potential of liquid-infused surfaces to reduce hydrodynamic drag, as a function of factors such as surface structure and level of infusion. This approach will allow us to quantify interfacial slip on liquid-infused surfaces within a custom-made microfluidic device. Results will be important for the fundamental understanding of drag-reduction and slippery nanostructured coatings.

**Supervisor:** Associate Professor Chiara Neto.

**A new family of self-assembled monolayers:** Our group has recently discovered a new family of self-assembled monolayers that can be formed on silicon and other oxide substrates, through nanoscale surface modification. This effectively turns the surface properties of glass into those of teflon, with very little effort. This discovery has opened the way to investigating a mechanism that is little studied in the surface science literature. We have so far established the conditions of formation, stability and uniformity of this monolayer, and we have just uncovered an important application. The monolayers have the ability to alter the work function of semiconductors, which could lead to more efficient photovoltaic cells.

**Supervisor:** Associate Professor Chiara Neto.

Please feel free to come and talk to me and members of my group for further information, or consult our Twitter (@ChiaraOz) and Instagram (netogroup) accounts.
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.
We investigate the fundamental question of how macroscopic properties emerge from nanostructure and dynamics of various forms 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, 6357–6426.) Deep eutectic solvents are cousins of ILs that consist of ionic and non-volatile molecular components. We are exploring the origins of their nanostructure, and using this knowledge to design new kinds of liquids and soft materials. We make extensive use of advanced neutron and X-ray beam techniques in our laboratory and at major international facilities, complementing NMR, microscopy and thermal analysis.

Novel amphiphilic liquids (2 projects): Recently it has been discovered that some metal complexes or solvates can stabilize of the liquid state, yielding new self-assembled or solvate ILs (SILs). In project 1 we will use amphiphilic ligands with metal salts to create new nanostructured liquids and liquid crystals with the advantages of conventional ILs. Of particular interest are lithium salts as novel electrolytes for batteries. **Supervisor:** Professor Greg Warr.

Deep eutectic solvents (DESs) are emerging as cheap and versatile alternatives to ILs, but very little is known about their liquid structure, and therefore about how to design and stabilise them. Starting with some of the best known and characterised DESs, and building on our detailed knowledge of ILs, in project 2 we will examine the effect of amphiphilic elements into DESs on their nanostructure and properties. **Supervisor:** Professor Greg Warr.

“Smart” ouzo: We have recently examined the structure of binary and ternary liquid mixtures that comprise aperitif liqueurs like Ouzo, which lies on the stability edge between microemulsions and emulsions, including replacing water with ILs. In this project we will design new liquids incorporating components that respond to light, temperature, salt concentration or pH to create responsive or switchable phase-transition materials. In doing so we will uncover how these structures form, and what features of the components structure are critical in determining stability. (J. Phys. Chem. B, 2014, 118, 9983–9990; J. Phys. Chem. B, 2015, 119, 5904–5910) **Supervisor:** Professor Greg Warr.

**Micelle or nanoparticle? You be the judge:** One of the most often forgotten things about a micelle is that it is an equilibrium object. Block copolymer micelles are often not micelles at all, but nanoparticles. To build new nanostructured matter we need to know when kinetics matters, and when we’re at equilibrium. **Supervisor:** Professor Greg Warr.

Dynamics are also critical for controlled release applications for drug, perfume or nutrient delivery. New polymer preparation techniques allow us to move continuously in synthetic space from small surfactants to 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 how to design, control and preserve nanostructured materials (Langmuir, 2014, 30, 7986–7992) **Supervisor:** Professor Greg Warr.

**Out there: How alien can alien life be?** The news frequently reports new exoplanets detected by the Kepler orbiting telescope, while the Cassini-Huygens mission revealed surprising features of the Saturnian system. Each new discovery is usually accompanied by speculation about whether life could exist in these alien environments, and whether they lie within 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 are met in nanaqueous environments such as the ethane lakes of Titan or in 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.

Please feel free to contact me to learn more about these and other projects available.
As part of the Centre of Excellence in Exciton Science, we use mathematical modeling and computer simulations to understand the behavior of existing materials and to design new materials for solar energy capture, sensing, and catalysis. 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 at interfaces 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 interfaces and molecules bound to the particle surface can be used to assemble such nanorods 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 the Centre of Excellence in Exciton Science to create such assemblies in the laboratory. Supervisor: Dr Asaph Widmer-Cooper.

Using molecular hairs to 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 to investigate this order/disorder transition and how it affects the optical properties of the particles. This may involve interaction with experimental collaborators in Melbourne and Germany. Supervisors: Dr Asaph Widmer-Cooper and Dr Girish Lakhwani.

Nucleation and growth of metal halide perovskites: 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 molecular interactions that control their nucleation and growth. In this project, you will use computer simulations to study how metal halide perovskites nucleate and grow in solution, in collaboration with our experimental partners from the Centre of Excellence in Exciton Science. Supervisor: Dr Asaph Widmer-Cooper

Porous nanoparticle superlattices for catalysis and sensing: Nanoparticles can now be made with exquisite control of shape and are becoming increasingly important as building blocks for new high-tech materials. Mixtures of particles with directional interactions are attractive candidates for making a new family of porous superlattices, with potential applications in catalysis, sensing, and optics. You will explore the range of assemblies that can be made by extending a structural search algorithm and using Monte Carlo simulations. Interesting structures may be synthesized by experimental collaborators in Japan or the USA. (see Nature Materials, 2012, 11, 131-137). Supervisors: Dr Asaph Widmer-Cooper and Dr Toby Hudson.

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 A/Prof Chiara Neto. Supervisors: Dr Asaph Widmer-Cooper and A/Prof Chiara Neto.

Phase behaviour of Janus rods and helices: Nanoparticles can now be made that have surfaces with two distinct physical properties. Such Janus particles can exhibit complex phase behaviour ranging from small micelle-like clusters to sheets and twisted assemblies. This provides a scalable way to assemble complex nanostructured materials with unique properties. In this project, you will use computer simulations to investigate the phase behaviour of Janus rods and helices, which will allow you to discover how their phase behaviour differs from those of Janus spheres, hard rods and hard helices. Supervisors: Dr Asaph Widmer-Cooper and Dr Toby Hudson.

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
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 cannabinoid agonists and antagonists were found to improve target selectivity, in vivo potency, and pharmacokinetic profile. This project is in collaboration with A/Prof. Jonathon Arnold (Pharmacology).

Phytocannabinoid derivatives as GPR55 antagonists: The cannabis plant produces more than 100 unique molecules, with two cannabinoid approved for clinical use; Marinol® for chemotherapy-induced nausea and vomiting, and Epidiolex® for Dravet syndrome. Despite in 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).

Peripheral-restricted cannabionoids ligands: Cannabionoid receptors are expressed abundantly throughout the brain, but also in the periphery. The clinically-approved cannabionoid antagonist rimonabant was withdrawn from the market owing to adverse effects associated with its central nervous system penetration (CNS), while brain-permeable cannabionoid agonists like tetrahydrocannabinol produce intoxication. By rational modification of the lipophilicity, polar surface area, and number of hydrogen bond contributors, we have developed several cannabionoid agonists and antagonists with limited ability to cross the blood-brain barrier. Peripherally-restricted cannabionoids 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 cannabionoid 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-ethylpentylene), 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. Ray 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/
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: Cameron is a teenage boy living in Brisbane. One day he got the flu; next morning he woke up with a rare form of Parkinson’s disease, rapid-onset dystonia Parkinsonism (RDP). Now he needs to be fed through a tube because he can’t control his tongue movements. This cruel disease, which is triggered by physical or emotional stress, is caused by a mutation in the α3 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 the mutation responsible for the development of RDP. 

Supervisor: Associate Professor Ron Clarke.

Batten’s disease: 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. Emily is an eight year old girl living in Sydney who unfortunately has inherited Batten’s disease from her parents, who are both carriers of the recessive Batten’s disease gene. Due to the gradually accumulating damage her nervous system has suffered, Emily is now already almost totally blind. 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 researchers in the USA showed that treatment of battenin-deficient mice with the sterol carbenoxolone caused a reduction in disease symptoms. It was proposed that this is due to carbenoxolone binding to the lysosomal membrane and 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 such as Emily.

Supervisor: Associate Professor Ron Clarke.

Please feel free to contact me to learn more about these and other projects available.
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 safety 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 [11C]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 [11C]DPA-713) have been developed in recent years, but by and large suffer from undesirable binding affinity variation with 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.
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:** 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:** Professor Kate Jolliffe.

**Anion sensing in biological systems:** Phosphate anions, such as ATP, cAMP and pyrophosphate, are essential in biological processes, and imbalances in levels can be a cause or effect of disease. For example, pyrophosphate levels in synovial fluid are much higher in arthritic than in healthy patients, while thiamine pyrophosphate levels are a marker of Vitamin B1 deficiency. Despite their importance, there is a lack of simple techniques for selective measurement of one phosphate anion over another. This project will involve harnessing the potential of fluorescent anion receptors to develop simple protocols for studying phosphate anions in biological systems. This will suit students with interests in the use of NMR, UV-vis and fluorescence to study supramolecular systems, and can include synthetic and/or biological studies. **Supervisors:** Professor Kate Jolliffe and A/Prof Elizabeth New.

**Fluorophore labelled cyclic peptides for exploring biological function:** Cyclic peptides display a wide range of biological activities and cyclisation of a peptide can lead to ligands that bind more tightly and specifically to their protein targets. By attaching a fluorophore to these bioactive molecules we can better understand their biological function. This project will explore tagging the cyclic peptide oxytocin with a variety of fluorophores to explore whether oxytocin plays a role in the development of prostate cancer. This project will suit students with an interest in synthesis and biological studies. **Supervisor:** Professor Kate Jolliffe.

**Near infra-red dyes for optical sensing:** Dyes and fluorophores that absorb and emit light in the near infra-red window of the electromagnetic spectrum are highly desirable for applications in sensing, particularly in biological applications. In this project you will synthesise new near IR dyes, investigate their photophysical properties and use them to fabricate sensing devices. This project will suit students with an interest in both synthesis and the study of molecular properties. **Supervisors:** Prof Kate Jolliffe and Dr Girish Lakhwani.

**Anion scavenging systems:** In many industrial applications it is necessary to remove anions such as sulfate from both feed and waste water streams, but there are only a few ways of doing so and new methods are required. We have developed molecular receptors capable of binding to sulfate in aqueous mixtures and in this project will use these to functionalise polymers to provide systems suitable for scavenging sulfate from water. The project will involve aspects of polymer synthesis and characterisation together with analysis of the anion extraction ability of the functionalised polymers using a variety of techniques. **Supervisors:** Prof Kate Jolliffe and Dr Markus Muellner).

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

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

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

Supervisor: Dr William Jorgensen

(Possible dual supervision).

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.

Fig 1: A. Before stroke (normal brain), zolpidem modulates GABA by mainly activating synaptic α1ββ2 receptors (phasic currents) as they possess an α1-β2 interface. Zolpidem is inactive at extrasynaptic GABA ARs (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 GABAAR receptors such as (α1)3(β3)2 which possess an α1-α1 interface that only become present following stroke.

Bioisosteric amide replacement
Various heterocyclic analogues
Structural minimisation
Explore alternate linkers

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. Research in the Kassiou group utilises modern synthetic organic chemistry techniques for the rational design and synthesis of novel compounds for a range of CNS targets. The work in our laboratories has led to spin-off companies and first-in-human trials of drug candidates. The projects below are only a sample of what is offered, and projects can be tailored to suit the specific interests of any student.

Targeting protein aggregation:
Protein aggregation is associated with many disease states, in particular Alzheimer’s disease, Parkinson’s disease and frontal temporal dementia, among others. This occurs when proteins misfold and aggregate together, generally resulting in cell death. Our work tackles this problem on multiple fronts, developing small organic molecules that inhibit the processes that lead to misfolding, reduce aggregation and/or dismantle aggregates that have formed.

Tau-protein containing neurofibrillary tangles (NFTs) lead to a variety of tauopathies. Normally, tau binds to microtubules and facilitates microtubule assembly and stability. However when the balance between tau phosphorylation and dephosphorylation is changed in favour of the former, tau is hyperphosphorylated leading to aggregation and negative pathology. We are generating compounds that tackle this problem in two broad ways 1) by targeting the phosphorylation stage and 2) inhibiting or reversing tau aggregation. **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 and then neurodegenerative diseases. Our research is developing 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 appropriate for PET imaging. To achieve these goals, we are targeting one of three receptors: TSPO, P2X, and cannabinoid receptor 2 (CB2).

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 of these hurdles, displaying high specificity and a “one-size-fits-all” binding affinity regardless of genetic polymorphism. **Supervisor:** Dr Jonathan Danon, **Co-supervisor:** Professor Michael Kassiou.

The P2X receptor plays an essential role in inflammatory signalling as its activation leads to the formation and release of interleukin-1β (IL1β), a proinflammatory cytokine which plays a major role in the inflammatory pathways underlying neurodegenerative processes. Our work is developing ligands that bind to the P2X1 receptor at both the allosteric and orthosteric site to inhibit activation of this receptor. **Supervisor:** Professor Michael Kassiou.

Synthetic cannabinoids (SCs) are the most rapidly evolving class of widely abused “designer drugs”, and pose a major public health concern. However, they are also a great source of lead molecules that target the cannabinoid receptor. By making structural modifications to SCs we aim to synthesise compounds that selectively target the CB2 receptor and offer both a treatment and imaging option for neuroinflammation. **Supervisor:** Professor Michael Kassiou.

**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 is a 9-amino acid cyclic peptide that exerts prosocial effects in mammals through activation of the oxytocin receptor. However, it is far from ideal as a drug and not very brain permeable. This project will synthesise non-peptide oxytocin receptor agonists and elucidate structure-activity relationships. **Supervisor:** Professor Michael Kassiou.

Please feel free to contact me to learn more about these and other projects available.
Sensing lipid domains in biological membranes: This project is in collaboration with A/Prof. Elizabeth New. Molecules on the plasma membrane control the extent and type of conversations a cell has with its environment, and how the information is internalised and processed. This begins with the lateral separation of plasma membrane-lipids into two phases - liquid-ordered (Lo) and liquid-disordered (Ld) lipid domains. These domains are crucial for endosomal sorting of proteins, signal transduction, immune response and membrane trafficking. Disturbances in such highly regulated processes are observed in many diseases including muscular dystrophy, diabetes, hypertensions and neurodegenerative diseases such as Alzheimer’s and Parkinson’s disease. Due to the lack of sensors for lipid domains, membrane lipid-sorting has only been studied using fluorescently-labelled lipid analogues which exhibit different membrane behaviour compared to unlabelled ones. Therefore, these investigations have not been very successful.

This project aims at the design and development of molecular rotors that exhibit a change in their fluorescence properties, depending on the polarity and viscosity of their environment. Fluorescence microscopy and image analysis thereafter will provide a thorough understanding of the physiological role of lipid domains and their segregation, and facilitate the reliable diagnosis of physiological and pathological changes in cells.

Supervisor: Dr Amandeep Kaur and Co-Supervisor: A/Prof. Elizabeth New.

Understanding Alzheimer’s disease at the nano-scale: This project is in collaboration with Prof. Peter Rutledge. Protein misfolding and aggregation are hallmarks of many neurodegenerative diseases. In Alzheimer’s disease (AD) and frontotemporal lobar degeneration (FTLD), the amyloid-β, tau and TDP-43 proteins can be found assembled in amyloid fibrils, paired helical filaments or other aggregates where the morphology is less defined. A key question in this field is the nature of the differences between globular and fibrillar aggregates of these proteins. Standard optical techniques are limited by optical diffraction, examine ensemble behaviour and provide no insight into the structural details governing protein aggregation and its impact on other cellular factors. Therefore, an ability to visualise the molecular-level organisation, structure and distribution of proteins in these proteinopathies is central to gaining deeper understanding of the mechanisms underlying the associated neurodegeneration. This project involves the design and development of new amyloid-specific fluorescent probes with photophysical properties suitable for super-resolution imaging. The developed probes will then be applied to image the nano-scale organisation and distribution of aggregated proteins.

Supervisor: Dr Amandeep Kaur and Co-Supervisor: Prof. Peter Rutledge.

Super-resolution imaging: See what no one has ever seen before: This project is in collaboration with A/Prof. Elizabeth New. In recent years, super-resolution microscopy has revolutionised the study of biological and synthetic nanostructures by breaking the diffraction limit, and allowing visualisation of cells and materials on the molecular scale. While this Nobel Prize-winning technology demonstrates great potential for biomedical researchers wishing to unravel molecular-level interactions, the quantitative information obtainable and the progress in this field, are greatly limited by the small number and poor photophysical properties of existing fluorophores. An often-cited quote from Nobel Prize winner, Eric Betzig, who in his work on super-resolution microscopy constantly needed to “beg chemists for better probes”, further emphasises the need for new fluorescent probes with improved properties. In this project you will be working towards the design and synthesis of molecular sensors with super-resolution properties. With the use of cutting-edge super-resolution microscopy techniques, you will be applying the developed sensors towards visualising biological events and processes below the diffraction limit of light.

Supervisor: Dr Amandeep Kaur and Co-Supervisor: A/Prof. Elizabeth New.
Nature is full of remarkable nanoscale machines that can walk, talk, bind and self-assemble. As synthetic chemists, we have the opportunity to borrow from nature's vast catalogue of biomolecules, and modify their properties to create synthetic macromolecules that can perform completely new functions – cancer drugs, smart materials and nanostructured catalysts.

Our research projects are very diverse! You can choose from projects that cover a wide range of techniques: organic synthesis, protein engineering, DNA design, microscopy, cell culture, biophysical assays, and peptide chemistry.

Self-assembling nanocompartments for next-generation catalysis: Nature is a master of self-assembly, constructing functional nanoscale architectures from simple protein building blocks. Using synthetic chemistry, we can harness the power of self-assembling proteins to create new catalytic architectures.

This project involves chemical modification of encapsulins, bacterial proteins that spontaneously assemble into hollow ~30 nm shells (see Nat. Commun. 2018, 9, 1311). We will create nanoscale reaction vessels by functionalising the interior of these shells with enzymes and synthetic catalysts. Collaborators include A/Prof. Stephen Bell (Adelaide) and Prof. Marcela Bilek (Physics).

New biocompatible reactions for protein modification: Site-specific modification of proteins is a major challenge for synthetic chemists. This is a question of chemoselectivity: how can we perform a reaction at a chosen functional group, without affecting the hundred other unprotected groups that exist on a protein?

In this project, we will develop new organic chemical reagents that only react with a chosen function group in a specific amino acid sequence. The project will involve reagent synthesis and screening for reactivity against different peptide sequences. These reagents will enable us to label proteins in cells to study their roles in disease, and synthesise antibody-drug conjugates with improved efficacy.

Building synthetic life: Life is defined by compartmentalisation. All living things build compartments, each with a unique environment for hosting different chemical reactions.

In this project, we will create synthetic modified versions of the encapsulin family of self-assembling proteins (see Nat. Commun. 2018, 9, 1311) to create compartments with unique chemical properties within their interior. The ultimate goal is to generate new living organisms that possess artificial organelles with programmable chemical functions that are new to nature. This project is in collaboration with Dr Tobias Giessen (Harvard/ Michigan, USA).

Anti-cancer peptide therapeutics: Macrocyclic peptide-based compounds are highly-underexploited molecule in drug development. Peptidic macrocycles can have exquisite selectivity and potency similar to protein drugs, and pharmacokinetics that are normally associated with small molecules.

In this project, we will establish a new strategy for synthesising vast libraries of macrocyclic ‘stapled’ peptides, using a combination of bioorthogonal chemistry and recombinant technologies (see Angew. Chem. Int. Ed. 2015, 54, 15410-15413). The resulting compound library will then be screened in cellular and in vitro assays to identify new anti-cancer drug candidates.

Co-supervised projects: We have a range of joint projects! Full details are on our group website.

Bio-templated inorganic and polymeric nanomaterials (with Dr Markus Muellner): We can use biology to produce self-assembled structures that are incredibly uniform and precise, beyond what is possible using conventional synthetic techniques. Nanoparticles with new catalytic and structural properties will be templated by bacterial encapsulin nanocompartments.

Anion-binding gates for biomolecular cages (with Prof. Kate Jolliffe): We will use anion-binding as gates for self-assembled protein cages. By binding to the pores of the cage, we will control the ability of small molecules to enter and exit these molecular cages, enabling new forms of selective catalysis and drug delivery.

Please feel free to contact Yu Heng to learn more! Full project details are also on our group website: http://groups.chem.usyd.edu.au/lau/honours.html
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 analogues 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 organochemistry, 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 institutions. Supervisor: Peter Lay.

Please feel free to contact me to learn more about these and other projects available.
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. The primary attrition is the intolerance of drug-related side effects. Recently, there is a considerable interest in the development of natural products extracted from healthy diets for cardiovascular-protective therapeutics owing to the inherent safety profiles and the clinical evidence for ameliorating drug-induced cardiotoxicity. However, it remains a huge challenge to understand the protective mechanisms at the molecular level, which impedes pharmacological optimisation of these bioactive agents for therapeutic use. Therefore, we aim to apply cutting-edge chemoproteomics platforms to understand their intricate biological functions in cardiomyocytes and platelets and construct a comprehensive chemical genetics’ database for cardiovascular-protective drug discovery.

Sulforaphane and alliin are known to be the cardioprotective “ingredients” in broccoli and onion diets. They have been shown to promote cardiomyocyte survival against ischemic injury and exhibit potent anticancer activities. However, the protein target spectra of these small molecules in cell remain unclear. There is no generic model to explain the phenotypes observed in the treatment. Therefore, the specific objectives of this honours project are to:

1.Chemically synthesise sulforaphane and allin-based proteomic probes.

2. Profile the target spectra of sulforaphane and allin in cardiomyocytes, platelets and cancer cells to comprehend the understanding of the modes of action in living system.

3. Establish and optimise combination therapy for cancers involving sulforaphane and allin with a view to increase the efficacy and mitigate cardiotoxicity. 

   Supervisor: Dr Xuyu Liu.

Chemical synthesis and phenotypic validation of precision proteolysis targeted chimeras (PROTACs) for cancer and cardiovascular disease: The Akt kinases are critical regulators of cell physiology but have also been associated with the development of thrombosis, cancer and other biggest killer diseases. Recently, the revolutionary approaches in drug development termed PROTAC (PROteolysis-TArgeting Chimera) have attracted considerable attention in repurposing broad-spectrum therapeutics to be target-selective degraders. PROTACs are bifunctional molecules capable of binding to a ubiquitinase complex and the protein target simultaneously, thereby promoting selective target degradation. Importantly, rational design of PROTAC constructs has led to isoform-specific degraders to target oncogenic kinases and transcription factors otherwise intractable to functional inhibition.

This honours project aims to develop Akt-isoform-specific PROTACs and to investigate their therapeutic potential in thrombosis and cancer. The specific objectives of the project include:

1. Rationally design and chemical synthesis of Akt-isoform-specific PROTACs.

2. Phenotypic validation of PROTAC efficacy and selectivity in cancer cells and platelets.

3. Investigating the spectrum of targeting of PROTACs using modern chemoproteomic technologies to understand Akt isoform function in cancer cells and platelets with a view to developing new therapeutics. This project will be co-supervised by: Dr Xuyu Liu and Professor Richard Payne (School of Chemistry).

Please feel free to contact me to learn more about these and other projects available.
**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, maftotoxin 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 underpinning 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.

**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.
Our research spans chemical education, science communication and outreach to understand how we can better teach, communicate and improve public awareness of the chemical sciences. The following are outlines of some possible projects, but please feel free to contact Alice to discuss other research opportunities.

**Breaking good – Citizen science and drug discovery:** Drug discovery is traditionally a highly secretive process. Open source drug discovery aims to find new medicines more efficiently by sharing data and ideas. Removing secrecy from this process has enabled us to engage high school and undergraduate students in drug discovery. The Breaking Good Project works with junior students on the synthesis of medicines that aren’t accessible to patients; either because the market incentive is insufficient to motivate their discovery or because existing medicines are unaffordable. 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.

In this honours project, you will investigate the pedagogical importance of practical demonstrations in science education and use contemporary chemical educational literature to inform your research into safe, suitable and effective demonstrations for diverse audiences. **Supervisor:** Dr Alice E Williamson **Co-supervisor:** Associate Professor Peter Rutledge.

**Building a modern chemistry set:** Chemistry is a practical subject and hence experiments and demonstrations form an essential part of chemical education. Outside of specialised institutions - such as university chemistry departments - some chemicals or equipment are not available and limitations surrounding health and safety can restrict the use of certain reagents. Additionally, classroom teachers may lack preparation time or appropriate training to conduct demonstrations.

In this honours project, you will develop process-style chemical synthesis that is suitable and safe for high school laboratories and research the best way to teach synthetic organic chemistry to citizen scientists. **Supervisor:** Dr Alice E Williamson.

**Does chemistry have an image problem?** Chemistry is the central science and a core subject for numerous degree programs including medicine, agriculture, veterinary science and branches of engineering. Despite its central and pivotal role in society, representations of chemistry in the media are often linked to negative news stories such as explosions, chemical spills or pollution. The Royal Society of Chemistry have probed public attitudes to chemistry in the UK through a national in-depth study. While some findings from the report were positive – people are positive about chemistry’s contribution to society and indeed, public perception of chemistry is more positive than expected by chemists – the report found that people generally lack an emotional connection to chemistry and that most people can’t think of chemistry beyond their school memories.

In this honours project, you will explore whether public attitudes to chemistry in Australia mirror those found in the UK and investigate representations of chemistry in the media to examine any connection between perception and representation. The project will use databases such as Factiva to collate articles, TV programmes and radio segments that have included chemistry stories and analyse whether they have been correctly categorised and assess content sentiment. For pieces with the greatest audience reach, you will examine whether the content is accurate and effectively communicated for a general audience. **Supervisor:** Dr Alice E Williamson.

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

Studying oxidative stress in biology: Oxidative stress, which arises from imbalances of oxidising species and antioxidants within cells, has been implicated in many diseases of aging, such as cancer, cardiovascular disease and neurodegeneration. In order to better understand these relationships, it is important to be able to observe oxidative stress within cells, tissues and whole animals. In this project, we will design and synthesise new fluorescent sensors for oxidative stress, and then use these probes to study disease models. **Supervisor:** A/Prof. Liz New.

Fluorescent sensors for metal ions: Almost all biological processes require metal ions for correct functioning, particularly as cofactors in many enzymes. If metal levels are too low, enzymes will lose function, but if they are too high, incorrect metal complexes can form, leading to diseases like Alzheimer's. We will design fluorescent sensors for metal ions such as Ni(II), Mn(II), Cu(I) and Cu(II) that will allow us to understand the roles of metals in disease. **Supervisor:** A/Prof. Liz New.

Environmental monitoring of heavy metals: Years of global industrial activity has left residual pollutants, such as heavy metals, in the environment. It is important to be able to monitor heavy metal levels at remote locations, and therefore portable and simple technologies are required. In this project, we will explore fluorescent sensing techniques for measuring heavy metal levels, which can be applied to portable technologies. In particular, we will utilise array-based technologies, which can concurrently screen multiple samples and analytes. **Supervisor:** A/Prof. Liz New.

New fluorophores 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. The development of new fluorescent sensors is hampered by the limited number of suitable fluorescent scaffolds, particularly those that emit in the red or infrared. Projects in this area will involve identifying how new fluorophores can be made or existing fluorophores modified to improve the photophysical and biological properties. These projects will suite 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.**

Using 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. 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.**

Structure-property relationships in chiral fluorophores: Chiral fluorophores are an important class of compounds for molecular recognition, optical sensors and electroluminescent light emitting diodes (LEDs). High dissymmetry ratio, (i.e., differential sensitivity towards left (L-) and right (R-) circularly polarized light), good quantum yield, solubility, self-organization into supramolecular complexes are desirable parameters for their applications in the field of organic electronics and biological imaging. The aim of this project is two-fold – firstly, to design and synthesize new class of high quantum yield chiral fluorophores and secondly, to characterize them using various chiroptical spectroscopic techniques such as circular dichroism (CD) and circularly polarized luminescence (CPL). The project offers the opportunity for synthesis, computational modelling 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.
Tuberculosis and malaria drug discovery: Tuberculosis (TB) and malaria represent two of the most deadly infectious diseases, responsible for approximately three million deaths per year (1 person every 7 seconds). New drugs are desperately needed for these diseases due to the rapid emergence of drug resistance. Several projects are available which use a combination of synthetic organic chemistry, computer-aided drug discovery and drug screening technologies to develop novel small molecule inhibitors against validated target enzymes essential for the growth of the bacterium (in TB) and the parasite (in malaria). These compounds will serve as TB and malarial drug leads. The TB drug discovery project is jointly supervised by Professor Warwick Britton, Centenary Institute. The malaria drug discovery project is in collaboration with Professor Philip Rosenthal, University of California, San Francisco. Supervisor: Professor Richard Payne.

Synthesis of glycopeptide-based 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 glycopeptide segments of cancer-associated cell-surface glycoproteins. These will be covalently linked to immune-stimulating molecules to elicit a favourable immune response (see vaccine structure below). These molecules include a foreign peptide to stimulate T-cells (a T-cell helper epitope) and an immunoadjuvant (a lipopeptide which stimulates pattern recognition receptors on human cells). 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. This project is jointly supervised by Dr Scott Byrne, Sydney Medical School, The University of Sydney. Supervisor: Professor Richard Payne.


Chemical synthesis and phenotypic validation of precision proteolysis target chimera (PROTAC) for cancer and cardiovascular disease: The Akt kinases are critical regulators of cell physiology but have also been associated with the development of thrombosis, cancer and other biggest killer diseases. Recently, the revolutionary approaches in drug development termed PROTAC (PROteolysis-Targeting Chimera) have attracted considerable attention in repurposing broad-spectrum therapeutics to be target-selective degraders. PROTACs are bifunctional molecules capable of binding to a ubiquitinase complex and the protein target simultaneously, thereby promoting selective target degradation. Importantly, rational design of PROTAC constructs has led to isoform-specific degraders to target oncogenic kinases and transcription factors otherwise intractable to functional inhibition.

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3. Investigating the spectrum of targeting of PROTACs using modern chemoproteomic technologies to understand Akt isoform function in cancer cells and platelets with a view to developing new therapeutics. This project will be supervised by: Professor Richard Payne and Dr Xuyu Liu (School of Chemistry).
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 chemistry.

**Carboranes as unique boron frameworks 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 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. **Supervisor:** Professor Lou Rendina.

**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 Gd³⁺ 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, the first time that GdPAT experiments have ever 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. **Supervisor:** Professor Lou Rendina.

**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 (photon activation therapy (PAT), neutron capture therapy (NCT), and targeted radiotherapy) and also in tumour diagnosis (PET and MRI) involving a variety of medically-relevant metal ions (e.g. Gd³⁺, Ga³⁺, and Lu³⁺).

**New boron-based epigenetic inhibitors for the treatment of malignant cancers:**

Epigenetics (and the so-called “epigenetic code”) will undoubtedly play an important role in future drug design and, indeed, several drug companies are now actively searching for small molecule epigenetic inhibitors for diseases such as cancer. These drugs can block critical pathways associated with, for example, DNA methylation and histone modification such as acetylation. A small number of epigenetic inhibitors have recently been approved for use in humans for the treatment of selected cancers including cutaneous T-cell lymphoma (CTCL). In this project, we will exploit boron in the design of small molecules that can inhibit epigenetic enzymes, e.g. histone deacetylase (HDAC) and histone lysine demethylase (KDM), for the treatment of malignant cancers. **Supervisor:** Professor Lou Rendina.

**New boron fluorophores for near-IR biological applications:**

Fluorescently-labelled molecules are invaluable tools in microscopy. There is an urgent need to develop new fluorophores, particularly those that emit in the near-IR, and those in which chemical properties can be easily tuned. This project will involve the rational design and synthesis of new boron-containing fluorophores, followed by photophysical characterisation and biological studies. **Supervisors:** Professor Lou Rendina and Associate Professor Liz New.

**Carborane-containing polymers as advanced materials:**

Carborane clusters have seen little application to date in an industrial context and their exploitation will undoubtedly lead to a profound transformation of those industries focussed on advanced materials. Indeed, new functional materials based upon these unique framework structures containing boron can be envisioned in polymer science. This project will largely focus on designing and synthesizing new monomer units incorporating carborane scaffolds for application in functional materials including hydrophobic and heat-resistant polymers, drug delivery systems, surface modifiers, etc. **Supervisors:** Professor Lou Rendina and Dr Markus Muellner.

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 or visit our group website to learn more about these and other projects available.
Research in the Rutledge group uses the tools of organic synthesis and chemical biology to develop new antibiotics and cancer drugs, create biologically-inspired catalysts for important synthetic transformations, and design chemical solutions to environmental problems.

Metal ion sensors for biology, medicine and the environment / Sensing with smartphones: Metal cations like Zn(II), Cu(II) and K(I) play a range of important signalling roles in the body. We are developing fluorescent sensors to image these metal ions inside and just outside cells as new tools for diagnosing diseases like diabetes, cancer and Alzheimer’s. We have recently reported a zinc sensor with ten-fold a brighter signal response to zinc(II) and a copper sensor that functions selectively in doped aqueous saline solutions. Now we are working to: develop new ways to combat resistant bacteria:

1. ‘double-punch’ and ‘resistance-activated’ antibiotics;
2. cyclobutanone analogues of traditional β-lactams (see ChemBioChem) as β-lactamase inhibitors;
3. new antimycobacterial agents with unprecedented structures and high potency against Mycobacterium tuberculosis and M. avium (collaboration with Prof Matthew Todd (UCL) and Prof Jamie Triccas, (CPC));
4. screening natural product extracts for new antimicrobial activity against MRSA and M. tuberculosis (with Prof Jamie Triccas (CPC));
5. mining microbial genomes in search of new bioactive natural products (see Nature Rev. Microbiol. 509 13 (2015), with A/Prof Nick Coleman (SOLES)).

In parallel approaches we are applying a similar strategy to develop new sensors for the heavy metal pollutants mercury, cadmium and lead, for environmental applications (see Chem. Eur. J. 17 2850 (2011) or J. Organomet. Chem. 696 715 (2011)), and important biomedical markers such as glucose.

Working on one of these projects, you will develop skills in organic synthesis, spectroscopy, chromatography, coordination chemistry and fluorescence techniques, plus either nanotechnology (QDs) or photonics (smartphones/ optical fibres). Includes collaborative projects with Prof Matthew Todd (UCL) and Prof John Canning. Supervisor: Professor Peter Rutledge.

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

1. biocatalysis – developing the potential of our new biocatalyst for alkene epoxidation using directed evolution and gene knock-out strategies (collaboration with A/Prof Nick Coleman (SOLES));
2. biocatalysis – creating new bio-inspired catalysts for allylic amination reactions, nitrile hydration, DNA cleavage and peptide hydrolysis.

Working on one of these projects, you will use peptide synthesis and a range of spectroscopic methods to characterise the new systems, including 1H and 13C NMR and IR spectroscopy, mass spectrometry, EPR, XAFS and gas chromatography. You will also have the opportunity to conduct biological assays on the compounds you make/ isolate in association with our collaborators in the Charles Perkins Centre. Supervisor: Professor Peter Rutledge.

Biocatalysis and bio-inspired catalysis: The development of efficient methods to selectively functionalise C–H bonds (ie convert C–H bonds to C–O or C–N bonds) is an area of great interest in organic chemistry. Iron has great potential in this area due to its availability, affordability and ability to promote a range of oxidation reactions. We have recently reported a new biocatalytic system that converts simple alkenes to chiral epoxides (see Appl. Microbiol. Biotechnol. 97 1131 (2013)), and a range of “bio-inspired” catalysts that oxidise hydrocarbon substrates (see for example Tetrahedron Lett. 54 1236 (2013) or Org. Biomol. Chem. 10 7372 (2012) or convert nitriles to amides (see Molecules 19 20751 (2014)). Two project areas are offered in 2019:

- biocatalysis – developing the potential of our new biocatalyst for alkene epoxidation using directed evolution and gene knock-out strategies (collaboration with A/Prof Nick Coleman (SOLES));

Please feel free to contact me to learn more about these and other projects available.
Proteins are incredible biological molecules that coordinate a diverse list of impressive functions in living cells. My research employs a number of techniques at the interface of biology and chemistry to elucidate how novel protein systems, particularly those involving enzymes, work at a molecular level so that they can be rationally manipulated for use in the medicinal, food security and fine chemical industries. Current efforts are focused on characterising a new oxygen sensing system recently found in human cells, which is a potential drug target for cancer and cardiovascular disease.

Background - Oxygen (O₂) is a vital biological resource most prominently known for its role as the final electron acceptor in aerobic respiration and, as such, adequate molecular mechanisms are needed to maintain its homeostasis. One eloquent and efficient way this is achieved is through cellular O₂ sensors; enzymes with low affinity for the gas, which enable hypoxic (low O₂) responses to propagate when O₂ concentrations fall below a certain threshold. Recent work conducted in collaboration with researchers at the University of Oxford has identified a novel O₂ sensing enzyme in humans called cysteamine dioxygenase (ADO), knowledge of which may help us understand how mammalian cells adapt to hypoxia (see Science, 2019, 365, 65-69). Information on ADO could lead to therapeutic strategies to treat detrimental health conditions where O₂ delivery is impaired such as cardiovascular disease and cancer.

During their Honours year, aspiring researchers will learn and implement a number of important techniques spanning biology and chemistry to characterise ADO at a molecular level, ultimately aiming to determine its mechanism and facilitate the discovery of therapeutic compounds to influence its activity. Example projects are listed below but different directions of investigation may be available depending on interest.

**Determine the molecular structure of the ADO by X-ray crystallography:** Structural analysis provides unprecedented information on how a target protein preforms its function, highlighting the spatial and chemical arrangement of key elements, such as the active site of an enzyme, which can enable rational manipulation of the molecule, either through genetic or chemical intervention. During this project you will clone, purify and crystallise recombinant ADO protein so that the enzyme’s 3D structure can be determined by X-ray crystallography at the Australian Synchrotron. Results from this work will help direct inhibitor discovery.

**Identify inhibitors and/or enhancers of ADO activity:** To better understand the role of ADO in regulating cell responses to hypoxia, it would be beneficial to have chemical tools to specifically manipulate enzyme activity and these compounds could serve as therapeutic devices to treat health conditions where oxygen delivery is impaired, as stated above. Using peptide synthesis, the candidate will generate chemical analogues of ADO substrates and test their influence on enzyme activity using mass spectrometry (MS), mRNA display, a powerful technology that identifies binding partners from a large pool of cyclic peptides, can also be employed to find leads (see Curr Opin Chem Bio, 2015, 24, 131-138).

Dissect the contribution of nitric oxide on ADO activity: ADO is an O₂ sensor but nitric oxide (NO), an extremely reactive signalling gas, has also been shown to interact with the ‘N-degron’ degradation pathway that ADO regulates in vivo. During this project you will test the impact of NO on ADO activity, establish its effect on protein and/or substrate chemistry as well as determine any NO derived modifications using a variety of analytical methods including MS and NMR.

**Test the role of CDO in regulating the N-degron pathway and/or re-engineer its functionality:** Cysteine dioxygenase (CDO) is a homologous thiol oxidase found in humans with a role in cysteine metabolism. It is important to establish whether it can function as an O₂ sensor in the N-degron pathway alongside ADO. Using recombinant protein and peptide synthesis, candidates will analyse the ability of CDO to modify substrate sequences by MS and use mutagenesis to re-design the enzyme to fulfil an O₂ sensing role if no functionality is detected.

Please feel free to contact Mark for more information or to discuss the work.
Hierarchical assembly of DNA origami nanostructures: In DNA origami we fold up a long piece of single-stranded DNA into 3D nanostructures, with almost any shape we want. For example, a DNA origami nano-spring that was used to simultaneously measure force and position of the protein motor Myosin VI during stepping (Nat. Commun. 2016, 7, 13715).

This project focuses on hierarchical assembly of many DNA origami components into much larger assemblies. These nanostructures can act as versatile nanoscale ‘breadboards’ complex 3D arrangements of matter, which will be demonstrated using super-resolution fluorescence microscopy. Supervisor: Dr Shelley Wickham.

DNA nanopores to target bacteria: In this project we aim to design a DNA origami nanorobot that selectively destroys microbes, to address the global challenge of antimicrobial resistance. This goal is divided into three sections: targeting, signalling and destruction.

Lipid-binding DNA origami structures will be targeted to specific microbes with DNA aptamers. Signalling will involve designing nanostructures to communicate with one another to cooperatively destroy microbes, and destruction methods to explore include disrupting microbial membranes with lipid binding DNA nanopores. Supervisor: Dr Shelley Wickham.

Using DNA nanotechnology to understand thrombosis on medical devices: Thrombosis is the leading cause of medical device failure, and we still don’t understand the molecular causes of this. In this project we will build and use DNA nanotechnology tools to examine how proteins on a surface can trigger thrombosis.

An array of DNA nanostructures will be precisely arranged on a UV lithography patterned, plasma-treated surface. This array will be to scaffold coagulation proteins for in vitro microfluidic studies. This project is in collaboration with Dr Anna Waterhouse (CPC, Heart Research Institute) and Prof Marcela Bilek (Physics/Engineering). Supervisor: Dr Shelley Wickham.

DNA-directed control of membrane proteins: In complex organisms, membrane proteins perform many essential processes, including touch, sight, hearing and cardiac rhythm. However, we still don’t understand how membrane proteins interact with each other in complex ways to achieve this. In this project we will develop new in vitro models for studying membrane protein interactions, using DNA origami nanostructures. This project is in collaboration with Dr Matthew Baker (UNSW/Biology) and Prof Hagan Bayley (Oxford/Chemistry). Supervisor: Dr Shelley Wickham.

Collective behaviour in synthetic molecular motors: Nature uses swarming to achieve complex behaviour from the interaction of many simple units. Army ants link themselves together to form rafts and bridges, and neurons in a brain fire off signals that collectively create intelligence. We have made molecular ‘walkers’ out of DNA, which can navigate a maze (Nat. Nanotech. 2012, 7, 169). In this project we will make and test DNA nano ‘ants’, DNA walkers than work together, and use them to explore collective behaviour. Supervisor: Dr Shelley Wickham.

Using 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. Supervisors: Dr Shelley Wickham and Associate Professor Liz New.

Please feel free to contact Shelley to learn more! More details on projects and current research are also on our group website: https://sydnagroup.com/
Computational and theoretical, soft matter, and materials chemistry

Research area:
Computational and theoretical, soft matter, materials chemistry

- Professor Peter Harrowell
I am interested in understanding the ways collective order can occur in atomic and molecular liquids and solids and how these complex types of order can influence the dynamics of these dense phases. These questions form the basis of modern theoretical materials science. While most of these projects involve some level of computer programming, no experience with computers is assumed.

The role of hydrating waters in stabilizing supermolecular structure: One of the great organizing ‘forces’ in self-assembly is the interaction of solutes with water. The interaction between waters of hydration themselves can play just as important a role. In this project as student will use computer simulations to study how the interactions between water in the solvation shell of a model protein influence the structure and dynamics of the solvated molecule.

Simulating crystal nucleation: The nucleation of a crystal from the disordered liquid is a remarkable example of spontaneous self-organization. In this project a student will develop a novel computational approach to this problem in which the rare crystal fluctuations are ‘encouraged’ by applying biases for crystallization that involve minimal assumptions about what form the nucleus might take.

Adsorbate binding energy distributions on disordered surfaces: Many modern catalysts consist of disordered metal alloys. An important physical property of these surfaces is the distribution of adsorbate binding energies of gas molecules. There is little known about this distribution on realistic glassy surfaces or about how this distribution can be measured. In this project a student will use simulations to model a glass surface and use a probe molecule to model the thermal desorption process as a means of measuring the underlying distribution.

How does rigidity appear in a network glass-former on cooling? Silica glasses are typically modified by replacing some silicon ‘ions’ with monovalent cations like sodium to decrease the viscosity and so make the glass easier to work. Recent work in the group has established a new measure of the degree of rigidity in a liquid structure as it is cooled. In this project a student will use computer simulations to study how the addition of sodium ions influences how rigidity develops as the liquid is cooled into the glass.

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

Professor Peter Harrowell

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CHEMISTRY EDUCATION

Research area:
Chemistry (education focused)

- Dr Stephen George-Williams
- Dr Reyne Pullen
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.