Bachelor of Science (BSc)
BSc Advanced Science
BSc Medicinal Chemistry
Honours in Chemistry 2019
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WELCOME

The School of Chemistry at UNSW is one of the leading centres of chemistry research in Australia. Composed of close to 30 well-funded research teams, we are located in the following buildings on lower campus: Dalton (F12), Chemical Sciences Building (F10NA and F10), the new Hilmer Building (E10) and soon the Science and Engineering Building which is currently under construction. The School has state of the art research facilities that enable research spanning the entire breadth of chemistry. The UNSW Mark Wainwright Analytical Centre (MWAC) is co-located adjacent to the School of Chemistry (F10NA) and provides major research facilities that are unsurpassed internationally.

Research in the School of Chemistry can be classified in four strategic areas:
- Nanoscience
- Energy & Environment
- Medicinal Chemistry
- Catalysis & Industry

In each area our School has world-renowned scientists that make significant impact on international research, making an impact in areas diverse as medicine, the molecular sciences, chemical industry and materials science.

The School of Chemistry at UNSW has strong links to Australia’s professional body for chemists, the Royal Australian Chemical Institute (RACI) and the International Union of Pure and Applied Chemistry (IUPAC). It also has close ties with the American Chemical Society (ACS). Several research team leaders hold senior positions in the RACI, and the NSW state branch is located in the School. Professor David Black was the Secretary General of IUPAC from 2004 – 2011, and is the current Secretary General of the International Council for Science (ICSU). Professor Sir Fraser Stoddart (2016 Nobel Laureate) has also commenced research activities within the School.

The School welcomes applicants for Honours from students throughout the world, acknowledging that the Honours year is an outstanding introduction to research. We are confident that the wide range of research undertaken in the School provides applicants with a rewarding Honours year.
Professor Scott Kable (Head of School)
Dr Neeraj Sharma (Chemistry Honours Coordinator)
OVERVIEW OF HONOURS

This booklet provides details for students interested in undertaking an Honours year with a major in chemistry in either the BSc or BSc Advanced programs or undertaking a BSc Medicinal Chemistry (3992). If you are a BSc Nanotechnology (3617) student, please consult the specialised Honours booklet for your degree.

Is the Honours year worth the extra year it takes? The answer is certainly “Yes!” for many people.

- The response from potential employers in industry and the public sector is that they will employ a good Honours graduate over someone with a pass degree.
- Honours is necessary for anyone contemplating postgraduate study in chemistry.
- Honours gives you “hands-on” experience in tackling projects, and provides a rewarding finishing quality to your education.
- Honours provides you with experience at managing your own project, independence and time management skills.
- Most important of all, the Honours year allows you to work closely with the staff in the School of Chemistry, and it transforms the University for you into a very human organisation that has people who support you.

HONOURS IN THE SCHOOL OF CHEMISTRY

In 2019 the School of Chemistry offers Honours programs that are suitable for students enrolled in Science, Advanced Science, Medicinal Chemistry and Environmental Science. The School of Chemistry also offers projects for Nanoscience students and projects are also accepted in other streams which can be discussed with the respective coordinators. School of Chemistry researchers also supervise or co-supervise the equivalent of a Honours project with colleagues in the Faculty of Science and in other Faculties which are typically made in a case by case basis.

Within the School of Chemistry all programs involve a proportion of coursework. BSc. Science or BSc. Advanced Science students with a major in Chemistry enrol in BSc. Honours (4500). Assessment is based entirely on your record during the Honours year, during which students have the opportunity to demonstrate skills in both research and coursework.

In the UNSW3+ model, the streamlined access to Honours is shown in the figure below. Students enrol in 48 credit points, first term of Honours in CHEM4501, CHEM4502 and CHEM4506, followed by CHEM4518 in your second term and
CHEM4512 in your third term. Marks for all courses, your Honours year mark is provided at the end of course. Feedback is provided on progress throughout the course by both the primary supervisor and other researchers within the School of Chemistry. Although Honours can be started in any term, we would encourage students to plan for a T1 or T3 start for Honours.

Chemistry Honours with UNSW3+

Students log on to [https://www.science.unsw.edu.au/honours](https://www.science.unsw.edu.au/honours) to apply for Honours. Here students need to rank in order of preference 3 potential research supervisors.
WHAT DOES AN HONOURS YEAR ENTAIL?

The aim of the Honours year is to continue your development into a well rounded chemist and research scientist by exposing you to independent research, advanced courses in Chemistry and a broad range of fields in chemistry through your attendance at research seminars.

The original research project forms the main component of the Honours year. Staff members offer numerous projects in their field of research, some of which are suitable for Chemistry Honours. Students nominate supervisors in research areas that interest them. They then work on a project under the close supervision of an allocated supervisor for the duration of the Honours year. Student-supervisor allocations are made on the basis of student WAM and demand for specific supervisors. Every attempt is made to allocate students their preferred supervisor or supervisors. Supervisor selections - https://www.science.unsw.edu.au/honours

Basic research skills are developed in the 6 units of credit course CHEM4501 to prepare you for your research project; areas covered include writing a research proposal, presentation skills, research ethics and modern occupational health and safety requirements.

Advanced level lecture courses are designed to extend your knowledge and broaden your understanding of key branches of chemistry. Honours students must take 6 units of credit (CHEM4502) in which students undertake 3 short courses offered by the School of Chemistry. These are advanced level courses of what are offered in undergraduate studies. Typically 2 courses are offered every term and over the course of the Honours year you are required to take 3 of the 6 offered courses.

Research seminars are conducted throughout the year and are an important means of exposing Honours students to research conducted in the School and at national and international institutions. Attendance is compulsory and unsatisfactory attendance will result in reduction of your Honours grade.
ADMISSION

ELIGIBILITY

For admission to Honours in the School of Chemistry, it is expected that a student will have achieved a credit average of WAM over 65 and have a BSc (or BSc Advanced) with major in chemistry. Students with qualifications in other disciplines may also be eligible for admission.

Students who have completed pass degree requirements at a University other than UNSW, or who have already graduated with a pass degree from UNSW or elsewhere, may be eligible to undertake an Honours year in the School of Chemistry. In such cases, please contact the Honours Coordinator (neeraj.sharma@unsw.edu.au) for clarification.

In all cases, admission is subject to the formal approval of the Head of School.
HOW TO APPLY

- If you are eligible to enrol (see previous page), approximately **3 – 6 months before** you intend to start Honours, consult the School of Chemistry Research Booklet ([http://www.chemistry.unsw.edu.au/current-students/undergraduate/honours-research](http://www.chemistry.unsw.edu.au/current-students/undergraduate/honours-research)) to determine which areas of research interest you and discuss these with the relevant academic member of staff. **It is strongly recommended that you talk to all prospective supervisors in your area of interest (i.e. at least 3 potential supervisors).**

- A good working relationship with your supervisor is paramount for the success of your Honours year. The choice of project is also important, and you are advised to obtain as much information as possible before making your decision. Find out what exactly is involved and what would be expected of you if you were to undertake a particular project.

- Honours deadlines for supervisor selection can be found via the on-line portal ([https://www.science.unsw.edu.au/honours-apply](https://www.science.unsw.edu.au/honours-apply)). Before the due date for each term you are required to submit this form with at least **three** supervisor preferences. Rank your order of preference. You must have spoken to and been given permission by at least three supervisors prior to nominating them (**note**: a cross-check will be made with all nominated academics).

- The School will contact you via email to advise the outcome of your application for Honours.

**For further information and assistance, contact:**

Honours Coordinator, Dr Neeraj Sharma:
neeraj.sharma@unsw.edu.au
ASSESSMENT

The Honours degree is graded into Class 1, Class 2 Division 1, Class 2 Division 2, Class 3 or Honours may not be awarded (see below for grade boundaries).

Assessment is on the basis of performance in the various components of the course, including the research project and the formal course work. Note that in order to be awarded Honours, you must achieve a satisfactory performance (>50%) in each component (coursework and research).

CHEM4501 - 6 UoC Research skills

CHEM4502 - 6 UoC Coursework

CHEM4506, CHEM4512 and CHEM4518 - 36 UoC Research

- Thesis Grading Committee’s assessment of Thesis
- Thesis Grading Committee’s assessment of the Final Seminar
- Thesis Grading Committee’s assessment of the Defence
- Attendance at School Research Seminars

Research skills (CHEM4501 6 UoC – 12.5%): In order to adequately equip yourself for your research project, you are required to take CHEM4501 which will cover how to write a research proposal, presentation skills, research ethics, managing your research and occupational health and safety.

Course Work (CHEM4502 6 UoC – 12.5%): You are required to take three different short courses during your Honours year. Every term two of these courses are offered and are geared to be advanced level options of undergraduate knowledge. Details are available from the Honours Coordinator (Dr Neeraj Sharma). You will nominate the 3 courses typically when you commence Honours.

Research Component (CHEM4506, CHEM4512, CHEM4518 36 UoC - 75%): The research project is the distinctive feature of the Honours year. It is the major undertaking of the year and is both the most challenging and rewarding aspect of Honours.

Students work on original research projects conceived and overseen by a member of staff. While you will be instructed by your supervisor on the nature of the project and will be given guidance in how to conduct the project, it is expected that you will perform all experimental work independently. You will be expected to prepare and
analyse experimental results and work with your supervisor to identify and overcome any problems. At the completion of the year you will present a thesis detailing the background, aims, experimental procedures, results and future directions of your project.

**Research Proposal and Presentation:** To assist in the preparation of your thesis and to allow your writing style to be improved, you will also be required to submit a research report describing your chosen research project and a review of pertinent literature. You will also do a short presentation on the proposal and your project. This will be in the first term of your Honours year and written feedback will be provided for both aspects.

**Thesis Submission:** You will write your thesis and submit it during your third term in Honours with the dates made available on your first term. Your thesis is a significant portion of your Honours mark and should be read and edited by numerous people including your supervisor.

You are required to submit a final version of your thesis that incorporates the Thesis Committee’s comments to your supervisor and the School for completion of Honours. Failure to do so will result in your Honours grade being withheld. The thesis accounts for 60% of your research mark.

**Honours Seminar:** You will be expected to present your work at two seminars during your Honours year; one will be a short overview of your project in your first term which will be graded within your research skills component (see above); and a longer seminar detailing your results to be presented after submitting your thesis; this seminar is typically 15 minutes long plus up to 10 minutes for questions. It comprises 15% of your research mark.

**Oral thesis defence (viva-voce):** The thesis defence will be shortly after you have submitted your Honours thesis and presented your final seminar and will be a closed examination of around 20-30 minutes with a panel of experts. It will comprise 25% of your research mark.

**Attendance at School Research Seminars:** Attendance at School Research Seminars is compulsory.

**HONOURS DEGREE GRADE BOUNDARIES (%)**

<table>
<thead>
<tr>
<th>Class</th>
<th>Percentage</th>
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<tbody>
<tr>
<td>Class 1</td>
<td>85+</td>
</tr>
<tr>
<td>Class 2 Division 1</td>
<td>75 – 84</td>
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<tr>
<td>Class 2 Division 2</td>
<td>65 – 74</td>
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<tr>
<td>Class 3</td>
<td>50 – 64</td>
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HONOURS
SUPERVISORS
DR. GRAHAM BALL  
Level 1, Dalton Building (F12)  
T: 9385 4720  E: g.ball@unsw.edu.au  

NMR SPECTROSCOPY AND COMPUTATIONAL CHEMISTRY:  
APPLICATIONS TO ORGANOMETALLIC AND BIOLOGICAL CHEMISTRY

Our research focuses on applying NMR spectroscopy to shed light on important chemical problems, often in the areas of organometallic and biological chemistry. NMR spectroscopy is probably the most powerful technique available to the chemist and the Mark Wainwright Analytical Centre is bristling with state-of-the-art instruments eagerly awaiting YOU to run experiments that push the boundaries!

Our experimental work is complemented and enriched by using computational techniques. We model small chemical systems with ab initio and DFT methods and biomolecular systems with molecular mechanics and QM/MM methods. This is a superb way to get detailed information about your molecules and their reactivity without all the risk assessments!

(a) Short-lived metal complexes and reactive intermediates

What should we do with petrol? Mostly it is just burned as fuel leading to damaging CO₂ and a rapid dwindling of this precious resource that took millions of years to form. Recently, chemists around the globe have been working on ways of converting relatively unreactive alkanes found in petroleum into useful compounds. A process known as C-H activation is at the core of these conversions, and we are studying the key short lived intermediates in this chemistry, which have an intact alkane molecule bound to a metal, to aid design of new catalysts.

These intermediates, known as alkane complexes, are generated by hitting precursor complexes with light while they are in the NMR spectrometer. Low temperatures are used to stabilise these reactive intermediates, permitting their characterization. With this strategy, we have observed several types of alkane complex¹,²,³ including the JACS cover above¹ and even complexes where xenon acts as a ligand.⁴ Alkanes contain no lone pairs for binding to the metal centre. Instead they bind using the electrons in the C-H sigma bond. This is why they are poor ligands and their complexes are so short-lived (~100 ms maximum lifetime at 25 °C).

**Designing new exotic molecules: Computational investigations of alkane and noble gas complexes**

We employ computational methods (DFT, ab initio) to aid the design and understanding of these fascinating compounds. For example, the recently observed cationic alkane complexes shown here were designed computationally prior to observation. Current projects are aimed at answering...
questions such as: Can we make more stable alkane complexes? Can we do chemistry with the alkanes when they are bound? What exchange processes do the alkane ligands undergo? Can we observe complexes with ligands that bind even more weakly?

Projects in this area can be primarily synthetically based (making new alkane complex precursors), NMR spectroscopy based (observing the new complexes and their reactions) or computationally based (designing new compounds and predicting their reactivity). The 3 components can be blended to suit the interests of students tackling the project.


(b) Anti-cancer drug-DNA interactions (in collaboration with A/Prof Larry Wakelin, School of Medical Sciences and Dr Don Thomas, NMR Facility)

DNA presents one of the most logical and practical targets for anti cancer therapeutics. We are investigating the binding of several bis-intercalating molecules that show promise as next generation anti-cancer drugs and also the binding of clinically established drugs such as mitoxantone. The solution structures of the DNA-ligand adducts are obtained via a suite of 2D NMR techniques coupled with NOE-constrained molecular dynamics simulations employing the AMBER forcefield. Our recent results have lead to a re-evaluation of how these bis-intercalators interact with DNA.5

The project involves a fusion of NMR spectroscopy and molecular modelling, at the molecular mechanics or QM/MM level. The project can be tailored to focus solely on NMR studies, solely molecular modelling or a balanced amount of both. We have a number of drugs synthesised that are ready for investigation.


(c) In silico studies of catalytic reductions (with A/Prof S. Colbran)

Building on the empirical results from A/Prof Colbran's group, we are modelling catalytic cycles of reductions of key small molecules such as CO2. Using density functional theory (DFT) allows us to get at the nitty-gritty of the mechanism of the catalysis and inform rational design of the next generation of reduction catalysts in this ARC funded project.

Supramolecular Chemistry

The use of weak, non-covalent interactions to form functional self-assembled architectures is core to my research interests, with a focus on metal-ligand bonds to direct the assembly of large multifunctional molecules, and light as a tool for chemical control.

**It would be great to work with Honours students on the following projects:**

(a) **Photoactive molecular cages**

(in collaboration with Dr Evan Moore, UQ)

Molecular cages are ‘small’ molecules with cavities capable of binding small molecules and anions. Within the confines of these cavities, usual reactivities can result, similar to the function of the binding pockets of nature’s enzymes. This project will involve using metal complexes as building blocks for cages capable of using natural visible light to catalyse reactions of bound substrates, the first example of which we published in 2015.[1]

Skills involved: organic and inorganic synthesis, multidimensional NMR, mass spectrometry, cyclic voltammetry, X-ray crystallography, photophysical measurements

(b) **Photoswitchable molecules**

(in collaboration with A/Prof Joakim Andreasson, Chalmers Institute of Technology, Sweden).

Some types of organic molecules can be isomerised between two forms using light. These two forms typically have very different properties, such as polarity, $pK_a$ and reactivity. We are looking to use visible light switchable molecules to control molecular reactions, such as driving pH changes or switching
ON/OFF catalytic activities. One example are spiropyran molecules, which act as ‘photoacids’, being switched between stable acidic and non-acidic states using light stimulus. Photoacids based on spiropyran may be directly incorporated into molecular and supramolecular systems for applications in stimulus-responsible switching with applications ranging from synthetic catalysis to in-situ drug release. New photoacidic molecules are required which are suitable for building into larger structures and membranes, and the tuning their photoswitching properties will be studied using a combination of spectroscopic techniques.

Skills: organic synthesis, multidimensional NMR spectrometry, mass spectrometry

(c) Novel ruthenium(II) complexes

Ruthenium(II) complexes are extremely useful complexes with applications ranging from energy storage and light harvesting, to catalysis and drug applications. This project will develop new types of chiral ruthenium(II) complexes which are responsive to their environments to allow these useful properties to be controlled by external stimuli (eg, temperature, chemical reagents, light, redox etc).

Skills: organic and inorganic synthesis, multidimensional NMR spectrometry, mass spectrometry, X-ray crystallography, cyclic voltammetry, X-ray crystallography, photophysical measurements

(d) Molecular rotors

(in collaboration with A/Prof. Jason Harper)

Being able to control motion at the molecular level is a fundamental challenge facing science. Nature uses controlled molecular motion, so called ‘molecular machines’ to control virtually every process in biology. So far, chemists use molecular machines to control nothing! This project involves the synthesis of molecular ‘rotors’ with a ‘propeller’ which can spin spontaneously when appropriate energy is supplied.

Skills: Organic synthesis, multidimensional NMR spectrometry

(e) …or other projects tailored to your interests!

• Clustering receptor proteins on the cell membrane can be used to control a range of cell behaviours. In my research I aim to design macromolecular architectures that can act as cancer therapeutics by clustering death receptor proteins on the cell surface.

• Because effective architectures are difficult to find by a rational design approach, I use combinatorial polymer synthesis to prepare and screen libraries of structures. Projects are therefore focussed both on the development of these combinatorial synthesis techniques, and on the use of them to design macromolecular therapeutics.

• I am a DECRA fellow within the school and work closely with the group of Prof. Martina Stenzel in the Centre for Advanced Macromolecular Design (CAMD) and with A/Prof. Adam Gormley at Rutgers University (NJ, USA). Please contact me for more information or to discuss any of the following projects.

It would be great to work with Honours students on the following projects:

(a) Combinatorial synthesis of star peptide-polymer conjugates for death receptor clustering (with A/Prof Adam Gormley, Rutgers University)

In recent years, triggering apoptosis through cell receptor clustering has emerged as one of the main targets for cancer chemotherapy, and a number of protein therapeutics that work through this mechanism are in clinical trials. However, natural proteins are not ideal therapeutics due to the difficulties in finding the right protein for any given application, their capacity to trigger immune detection and drug resistance, as well as their high cost and poor stability. Peptides that can bind to the relevant cell receptors are known and by presenting these on the surface of a scaffold we aim to design synthetic materials capable of clustering cell receptors with similar efficacy.

Polymers are attractive scaffolds to use for the presentation of these peptides as they allow precise control over architecture, density, and rigidity, as well as the position and number of binding moieties present. By synthesising libraries different architectures and measuring the relationship between their structure and biological efficacy, this project aims to design synthetic polymer-peptide conjugates for the clustering of death receptors on
breast cancer cell lines. The project will make use of new methods for oxygen tolerant polymer synthesis on microtitre plates that we have recently developed in order to prepare these libraries at low volume and high throughput.\(^2\)

The project will involve the synthesis of several chain transfer agents required to generate the different polymer architectures, the synthesis of peptides for receptor binding, and subsequent polymerisation and polymer analysis by NMR, GPC and associated techniques. Screening of biological activity will be performed in collaboration with Dr Adam Gormley at Rutgers University in the USA, and there is the possibility of visiting his lab in the middle of the year to perform some of this work if you so choose.

(b) Stabilisation of \textit{glucose oxidase} enzymes in nanocapsules \textit{(with Prof. Martina Stenzel)}

Despite their extensive use in a range of synthetic, biosensing, and therapeutic applications, enzymes are often highly unstable to heat, pH, and the presence of organic solvents. However, several recent studies have shown that it is possible to protect enzymes against degradation by such environmental factors by encapsulating them within nanocapsules.\(^{3,4}\)

We recently developed a new methodology for encapsulation of \textit{glucose oxidase} (GOx) inside a type of nanoparticle known as a polyelectrolyte complex (PIC) micelle. This gives excellent control over the structure of the nanoparticle, and allows us to crosslink the shell surrounding the enzyme to impart mechanical stability to the enzyme. In this project we will incorporate sugars such as trehalose, mannose, glucose and fructose, which have been shown to have a stabilising effect on enzymes,\(^3\) into our enzyme nanoparticles and compare their effects on enzyme stability. This will be done by first polymerising the sugars into the polymer backbone and then assembling them into the core of the PIC micelle. Enzyme activity will be monitored after exposure to a range of solvent, thermal, and other environmental stresses.

![Preparation of single enzyme nanogels. Adapted from Beloqui et al \(^2\)](image)

The project will involve controlled polymer synthesis and self-assembly techniques to prepare the enzyme nanocapsules, characterisation by light scattering and electron microscopy, and the use of enzyme activity assays to measure their activity under a range of environmental stresses.

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3) A. Beloqui, S. Baur, V. Trouillet, A. Welle, J. Madsen, M. Bastmeyer, G. Delaittre; \textit{Small}, 2016, 12, 1716–1722
Chen's research focuses on multidimensional carbon materials, particularly through the development of new synthesis strategies and applications. The core of Chen's research is the development of new synthesis strategies and understanding of properties of novel low-dimensional materials, especially carbon-based materials including graphene, graphene oxide, fullerenes, nanotubes, nano-onions, “peapods”, foams, foils and membranes, as well as relevant 2D materials and nanostructures.

It would be great to work with Honours students on the following projects:

(a) “Cooking” the “superstar” materials with domestic microwave

The microwave oven that we use to cook/heat food in the kitchen everyday can be used to prepare graphene – a single-layer of graphite and a “superstar” material in the current research field of materials science and chemistry. This Honours project involves the development of unconventional microwave induced shock processing of graphene and the preparation of graphene with various structures and properties. The synthesised graphene and related materials will be used in multiple applications, including energy storage, catalysis and sensing.

(b) Reconstructed two-dimensional materials for water separation

This Honours project aims to develop new types of membranes composed of stacked/overlapped layers of atomically thin sheets for selective separation of water through permeation. The project will involve the fabrication of membranes through van der Waals assembly of two-dimensional platelets with precisely controlled thickness, selective permeation of water through the membranes and studying the fraction processes using water analysers, and understanding water transport and permeation properties through confined nanometre-scale geometries in the membranes. This interdisciplinary research will seek new solutions to a major challenge in separation technology, which will be of significance for both fundamental and technological advances.

(c) Highly porous carbon made from “salt and sugar”

Is it possible to use “salt” and “sugar” to make new types of carbon materials with high electrical conductivity and ultrahigh specific surface area? This Honours project will explore the “magic” reactions between “salt” and “sugar” for preparing novel carbon nanostructures as well as selectively heteroatom-doped carbons, which are promising candidate materials for applications from electronics to energy.

I am open to discussions on other project ideas that you are interested in the “carbon playground”. Feel free to send me an email or just simply drop by my office.
Mass spectrometry is a core enabling technology that is used in many emerging and existing scientific fields. Dr. Alex Donald and his team are developing and applying experimental methodologies in mass spectrometry with a focus on problems in chemistry and biochemistry. We are looking for students who are interested in developing a valuable skillset in mass spectrometry and allied topics.

(a) **Significantly improving protein sequencing by mass spectrometry (w/ Dr. Junming Ho)**

A major goal in science is to comprehensively identify and quantitate all proteins in complex mixtures, such as the contents of cells, to rapidly facilitate biological and therapeutic discoveries. Because of the complexity and impressive molecular diversity of biochemical systems, this is an immense challenge. Several projects are available that broadly focus on developing and applying novel methodologies, instrumentation and theory in mass spectrometry to address this challenge.

To fully sequence an unknown protein, most current methods require the protein to be completely isolated from its biological matrix in high yield, which is time-consuming and can take weeks to months. In this project, you will work to develop methods that enable proteins to be sequenced faster with less sample. A significant barrier to improving protein sequencing by mass spectrometry is that protein ions, [Protein+2H]^2+, are normally formed in relatively low charge states (low z values), which do not readily fragment unlike those in higher charge states (high z values). This is a problem because the masses of the fragments are used to determine the sequence of the protein’s amino acids (i.e., the order and identity of the protein’s amino acids that are encoded by the protein’s gene). Moreover, the sensitivity and limit of detection of detectors significantly improve with increasing charge.

Supercharging agents are small molecules that are added to electrospray solutions to form protein and peptide ions in higher charge states than can be formed by other known methods. Recently, we set a new record for the most charge that can be packed onto a given protein ion by use of novel “supercharging” reagents (based on the propylene carbonate scaffold). This is significant because it enables a 65,000 Da protein to be sequenced in an experiment that takes less than 5 min and consumes less than 10^-12 grams of the protein; i.e., a feat that traditionally takes days and consumes significantly more sample. However, to apply this methodology to larger proteins, we must understand the mechanisms by which protein ions dissociate and the impact of high ion charge states on fragmentation so that performance can be improved further. In this project, you will learn valuable skills in computational chemistry and protein identification by mass spectrometry to elucidate the mechanisms by which gaseous protein ions dissociate so that ion fragmentation can be predicted. This information will then be useful for significantly improving protein identification by mass spectrometry.
(b) **Rapid, ultra-sensitive protein structure elucidation by mass spectrometry**

Potential drugs, pesticides, and antibiotics often fail because they bind to many proteins, leading to off-target side effects and safety issues. Pesticides and antibiotics can fail because of resistance resulting from changes to binding sites. This project will develop a method for rapidly discovering classes of molecules that bind to unique sites on proteins. This will provide scientists with novel starting points for designing new bioactive molecules aimed at improving effectiveness, safety, and preventing resistance.

The development of new pharmaceuticals is frequently delayed by the time and resources required to identify the sites that new chemical entities bind to protein targets. A recent breakthrough discovery in our laboratory has resulted in the ability to completely characterise large protein sequences directly from single mass spectra. This project aims to leverage this breakthrough by developing a rapid new approach for revealing ligand-protein binding sites using whole-protein mass spectrometry. The success of this project will enable novel sites of interactions between molecules and protein targets to be discovered rapidly and with high sensitivity. This will allow the efficient design of next-generation classes of bioactive molecules.

(c) **Cancer breathalyser**

Imagine a breathalyser test that can sniff out cancer and other diseases. The ultimate goal would be a personalised and highly accurate warning system for diagnosing disease in the earliest possible stages to maximise the possibility of recovery. This will require (i) high sensitivity, (ii) reliable detection, (iii) rapid sampling, and (iv) selective detection of many different types of molecules that are indicative of disease.

We have recently developed a compact ionisation method, called "surface enhanced ionisation," that can be used to directly ionise analytes from highly complex chemical mixtures without sample preparation for rapid detection by mass spectrometry. This is important because it eliminates chromatographic instrumentation which will significantly improve the performance of portable hand-held mass spectrometers by (i) reducing size and power requirements and (ii) increasing sensitivity and tolerance for complexmixtures.

In this project, you will use surface enhanced ionisation mass spectrometry to rapidly detect volatile organic molecules in breath and saliva that are "signatures" for lung and breast cancer with ultrahigh sensitivity. This project is part of a longer-term thrust towards developing a high performance portable, handheld, and personal mass spectrometer for monitoring/detecting disease and detecting harmful substances in your vicinity.
Chemistry plays a central role towards understanding the origins of life on Earth. My group seeks to develop experimental and theoretical models for understanding the potential chemistry that may have occurred on the Earth soon after its formation. Accomplishing this task requires a team with members who possess diverse expertise in synthetic organic, physical, analytical and biochemistries, aided by close collaborations with geo- and theoretical chemists. We are particularly interested in developing and understanding the chemical evolution of reaction networks that start from humble beginnings (i.e., small molecules thought to be available on the early Earth) and which yield complex mixtures that contain molecules of interest, such as amino acids, ribonucleotides and their precursors. From these humble beginnings, the further exploration of reaction network mechanisms for RNA and peptide polymerization can allow us to understand how Darwinian evolution may have come to take over chemical evolution.

I am a new Lecturer starting in the School of Chemistry, and expect to be able to take on students as early as T1 in 2019. Students may have potential opportunities to collaborate with and visit scientists from NASA Astrobiology labs in the US, as well as researchers from the Earth-Life Science Institute at the Tokyo Institute of Technology in Japan. Please feel free to contact me via email and schedule a meeting in person or online.

It would be great to work with Honours students on the following projects:

(a) Engineering Radiolytically Driven Reaction Networks

The need to make, measure and model complex reaction networks, especially those that give rise to hypothetically relevant prebiological compounds like ribonucleotides and amino acids, is fundamentally important for addressing the chemical mysteries shrouding life’s origins. The goal of this project is to utilize gamma radiation as an energy source to drive the evolution of an aqueous reaction network that begins with hydrogen cyanide (HCN) and which leads to building blocks for amino acids and ribonucleotides. We have shown already that a variety of compounds useful particularly for RNA synthesis – namely, cyanogen chloride, cyanalide, and glycolaldehyde – are produced in short order. Such a reaction network has the potential to serve as a model for better
understanding and engineering chemical evolution of complex mixtures in the laboratory that could have happened on the early Earth.

This project would require learning about organic synthesis, physical and analytical chemistries as well as modeling geochemical scenarios. Interested students are highly encouraged to contact me!

(b) **Understanding the Thermodynamics of Nonenzymatic RNA Replication**

RNA is often hypothesized to be among the first genetic polymers to have arisen abiotically from chemical evolution on the early Earth. The template-directed replication of RNA – without the aid of modern enzymes – offers a mechanism by which Darwinian evolution may have originally initiated. The objective of this project is to better understand the thermodynamics of the binding of ribonucleotide monomers and short oligomers to polymeric RNA duplexes. This initial step in the template-directed mechanism is made possible by specific noncovalent interactions, i.e., base-pairing. A quantitative understanding of such fundamental steps in nonenzymatic RNA replication is crucial for assessing whether this mechanism could have served reliably as a means to copy genetic information.

Those students who have a desire to become experts in solid-phase RNA synthesis, as well as supramolecular physical chemistry should definitely apply!

(c) **Testing Possibilities for Template-Directed Peptide Synthesis**

While potential mechanisms for nonenzymatic RNA replication are relatively well-understood, mechanisms for peptide copying on the early Earth that do not rely on modern biological enzymes are much less developed. A particular peptide that arises abiotically and happens to possess a useful function for a primitive cell could not evolve in a Darwinian fashion unless a reproduction mechanism existed. The goal of this project is to develop short peptides which self-assemble into highly symmetric nano-sized structures through reversible non-covalent interactions. These types of symmetric structures can serve as templates for the synthesis of their component peptides. Their reversible assembly ensures that molecular recognition of shorter oligomeric peptide fragments to unoccupied sites in the nanostructures can occur. Binding will preorganize these short oligomers for template-directed ligation reactions leading to the component peptide synthesis. This type of nonenzymatic template-directed peptide replication could lead to new avenues for understanding possible mechanisms for peptide evolution early in Earth’s history.

If you are interested in learning solid-phase peptide synthesis, as well as physical and analytical chemistry techniques, please schedule a meet!
Synthetic Organometallic Chemistry

- Research in the Field group is centred around synthetic organometallic chemistry:
  - Development of organometallic catalysts that are able to activate small molecules (such as N₂, CO₂, etc), functionalise organic hydrocarbons to make value-added products, and perform specific organic transformations.
  - Development of organometallic polymers for application in areas such as molecular electronics.
- Skills you will learn in the Field group:
  - Manipulation of air and moisture sensitive compounds.
  - Structure elucidation and determination of reaction mechanisms.
  - Heteronuclear NMR spectroscopy (³¹P, ¹⁵N, ²⁹Si, ¹⁹F), 2D NMR spectroscopy, IR spectroscopy and X-Ray diffraction.

It would be great to work with Honours students on the following projects:

(a) Organometallic Polymers

Organometallic compounds containing complexed metals linked by bridging groups have many potential applications in materials science. We are particularly interested in the use of alkyn groups as the bridging unit, and are developing new methods for forming metal complexes where the metal centres are bridged by organic acetyldes. Acetylde-bridged organometallic complexes show interesting electrochemical behaviour, and electronic communication between the two metal centres is often observed.

We recently discovered a straightforward route to an iron acetylide dimer where two iron centres are linked by a single C≡C bridge. We are interested in extending the chemistry to ruthenium and exploring the chemistry of C≡C bridged complexes. In particular, we are interested in extending the -M-C≡C-M-C≡C-M- chain to build up metal-acetylene polymers (seen in the figure below).
Alternative Bridging Groups for Organometallic Polymers

The majority of alkyne-bridged organometallic polymers use linear aromatic spacer units, such as 1,4-diethynylbenzene, as the bridge between metal centres. Non-aromatic bridges such as 1,12-diethynyl-\(p\)-carborane (C\(_6\)H\(_{12}\)B\(_{10}\)) have been described as “3D aromatic systems”. We are interested in the effect of aromatic bridges, as well as non-aromatic bridges such as 1,3-diethynylbenzene, on the chemical and electrochemical behaviour of organometallic polymers.

(b) The Organometallic Chemistry of Carbon Dioxide

Carbon dioxide reacts with many organometallic compounds to give products in which the CO\(_2\) is incorporated into the metal complex. A greater understanding of the ways in which CO\(_2\) binds and reacts with metal compounds may provide new ways to capture CO\(_2\) and utilise this wasted and environmentally dangerous compound.

Our previous work has focused on the stoichiometric insertion of CO\(_2\) into metal-hydride and metal-carbon bonds, to give metal formates and acetates, respectively. There have been many reports in the literature of catalytic activation of CO\(_2\) to yield formic acid (by hydrogenation), acrylates (by reaction of CO\(_2\) with ethylene), and carbonates (by reaction of CO\(_2\) with epoxides). We are interested in exploring the ability of novel iron(II) and ruthenium(II) complexes that we have prepared in the lab to catalytically activate CO\(_2\).

\[
\text{CO}_2 + \text{H}_2 + \text{Et}_3\text{N} + \text{ROH} \xrightarrow{\text{cat.}} \text{HCOOR}
\]

(c) The Chemistry of ‘CP\(_3\)’ Complexes

We have recently developed a new type of polydentate ligand for transition metals, which binds to metal centres using three phosphorus donors and an anionic carbon donor. To date, we have only explored the chemistry of this ligand on ruthenium(II). We anticipate that this ligand will form complexes with a wide range of transition metals, and are particularly interested in investigating the synthesis and catalytic properties of new rhodium and iridium complexes.

Selected publications from the group:

Recent progress in bioelectrochemistry has been linked to advances in our capability of mapping redox species on an electrified interface, a process commonly referred to as “electrochemical imaging” [1]. Addressing an electrochemical reaction with spatial resolution is usually done by the construction of electrochemical arrays [2]. However, a core principle of electrochemistry is that any electrode in an array must be connected to an external circuit via a wire such that either a potential can be individually applied to an electrode or an electrode potential can be monitored independently. There are two limitations of this requirement: (i) the connecting wire and associated bonding pads use considerable space on a chip surface and hence high-density electrode arrays are difficult to achieve; (ii) the position of each microfabricated conductive feature in an array must be pre-organized. A solution to these limitations was recently proposed in our published work on light-activated electrochemistry [3]. It was shown that a light pointer can selectively activate precise regions of a monolithic crystalline Si(100) electrode, such that electrochemistry can be performed where you want and when you want with a spatial resolution of 30 μm and just using a single-lead connection [4].

It would be great to work with Honours students on projects related to the following topics:

(a) Can we perform light-activated electrochemistry with improved spatial resolution? (in collaboration with Scientia Prof. Justin Gooding and Dr. Simone Ciampi / Curtin University)

The diameter of the active spot in light-addressable electrochemical devices based on semiconductors is determined by the size of the illuminated area (diameter of light beam) and the lateral diffusion of minority charge carriers. The former can be reduced by an appropriate optics but the latter remains the main challenge for achieving high-resolution electrochemical mapping. It is intended in this project to replace crystalline silicon by amorphous silicon and investigate the spatial resolution of the new light-addressable device. On crystalline silicon, transport of charge carries take place through motion in the extended states of the band. In amorphous silicon, on the other hand, the existence of band-tail states and electronic defects in the band gap change the transport mechanism to hopping between localized states. The consequence is the existence of traps for charge carriers, which minimize the lateral diffusion and improve the spatial resolution.

Cu2O based Mona Lisa electrodeposited on amorphous silicon by light-activated electrochemistry. [5]
(b) Can we combine Breath-Figure methodology and light-activated electrochemistry for “writing” multi-material arrays at nanoscale? (in collaboration with Scientia Prof. Justin Gooding, Prof. Richard Tilley and Prof. Susana Córdoba de Torresi / University of São Paulo, Brazil)

This project intends to “write” multi-materials on a silicon surface using light-activated electrochemistry. Combining multi-metal or multi-polymers on the same surface brings versatility to a range of electrochemical devices, such as sensors and surfaces for electrocatalysis. However, due to the reasons mentioned in item a, the utilisation of silicon has so far restricted the dimensions of the written materials to the micrometric scale. Here we intend to diminish this size by combining a nature-inspired methodology denominated “Breath Figure Method” with light-activated electrochemistry. Breath Figure refers to the fog (condensate droplets) that forms when water vapor contacts a cold surface. The common view is that the mechanism contains the following steps: (1) cooling of the polymeric organic solution and nucleation of the moisture, producing small but disordered water droplets on the solution surface; (2) growth and self-assembly of the water droplets, forming an ordered and closely packed water droplet array that covers the entire surface of the solution; and (3) evaporation of the solvent and water droplets, leaving a hexagonal pore array on the dry film. This is a methodology aimed for preparing a spin-coated porous polymeric mask to template the electrodeposition [6] of the multi-materials on a silicon surface and confine their dimensions of the writing materials to the nanometric size of the pore.

Our research group specializes in using self assembled monolayer or other surface modification technique to provide surfaces with unique functionality. The surfaces are the base upon which we build functional devices from nanscale component including polymer, protein, nanoparticles, and porous material. The three major programs in which these surfaces are applied are, biomaterials, biosensor, and drug delivery. The multidisciplinary nature of our research means we need people with interest in medicinal chemistry, surface chemistry, polymer chemistry, nanotechnology or analytical chemistry. All new members of the group will be looked after by a post-doctoral fellows as well as Prof. Gooding. Specific projects are:

Digital assays - Sensitive Biosensors for the Digital Age (in collaboration with Professor Richard Tilley)

The detection of disease biomarkers (such as proteins, DNA fragments and RNAs) in biological fluid is essential for the early detection of diseases. One of the primary challenges is the low concentration (typically in the femtomolar range) of the biomarkers. We are looking into new approaches to construct digital biosensors based on plasmonic nanoparticles. With the help of a dark-field optical microscope, we can look at the scattering arising from individual nanoparticles. The wide field nature of this measurement allows for the simultaneous characterization of thousand nanoparticles. When a biochemical sensing reaction is performed, the optical signature of the nanoparticle is altered thereby leading to change in the colour of the nanoparticle. By setting a threshold, we digitalize the data to 0 (unreacted) and 1 (reacted) nanoparticles. Our aim is to push this approach for the detection of individual biomarkers on individual nanoparticles.

Detection of Single Biomolecules using Magnetic Nanoparticles and Nanopore Sensors

A typical biosensors detects many molecules to give the concentration of species. Nanopores, which are commonly proposed for DNA sequencing, can detect single molecules and give concentration of species by counting many single molecules. This avoids the need for calibration however, detection limits are not as low as one expects because of the time taken for the molecules to find the nanopores. We have solved this problem by developing a new type of nanopore, referred to as a nanopore
blockade sensor. In this system, antibody magnetic nanoparticles capture the analyte of interest and bring it to the nanopore. The nanoparticle then blocks the nanopore to give a single molecule measurement. An additional benefit is the nanopore blockade sensors can operate in complex biological fluids. This project will involves developing the next generation of this exciting single molecule sensor.

**3D printing of cells for improved tumour models and drug assays (in collaboration with Australian Centre for NanoMedicine)**

Our current understanding of cancerous tumours is heavily based on in vivo experiments in animals or in vitro experiments on tissue culture plates. To date, few techniques exist that can satisfactorily recreate the tumour environment in vitro in 3-Dimensions. Such models would allow biologists to better understand the effect of spatial organisation of biomolecules on cell behaviour. Of particular interest are molecules that trigger cancer cell metastasis, or invasion, to other parts of the body. In our lab we are developing materials that can recreate the 3D tumour environment, made from polymers that provide a matrix for cells to attach to (see figure). In the proposed project, the polymers will be modified to include a peptide (protein-based) crosslink that stabilises the structure. Such protein-based regions are susceptible to degradation by specific types of enzymes (proteases) released by cancer cells when they invade surrounding tissue. The new materials developed in this project will be used as an extracellular matrix for the 3D printing of cells in collaboration with a 3D printing start-up company.

**The synthesis of electrocatalysts for fuel cells that mimic enzyme structure (in collaboration with Professor Richard Tilley)**

Electrocatalysts are important in applications as broad as fuel cells to sensors to production of fine chemicals. There are however a clear differences between a man made metallic electrocatalyst and a biological catalyst (an enzyme). In man made catalyst the catalytic sites are on the surface of the particle and the entire particle is conducting. However recent work in *Science* suggests catalytic sites in depressions may in fact be more active. In depressions or clefts are where most catalytic sites are located in enzymes. In this way the catalytic site is separated from the reactant solution which allows the chemical environment to be different from the bulk solution and the site to be protected from other species in solution. In this project we will synthesise catalytic nanoparticles for the oxygen reduction reaction that mimic enzyme structure by having the catalytic sites buried inside the particle but accessible via a small channel. Hence this work will focus on making core-shell nanoparticles, electron microscopy characterisation and performing electrocatalytic experiments with them.
Our research is focussed on understanding how organic processes happen and what affects reaction outcomes. Particularly this encompasses examining how structural features in both the reagents themselves and the solvent used can change how a reaction proceeds. This knowledge can then be applied to a range of fields, including bioorganic, synthetic, analytical and environmental chemistry. Being particularly interdisciplinary, there is extensive opportunity for collaboration and this is currently underway in the areas of catalysis, reaction kinetics, synthesis and molecular dynamics simulations.

a) Ionic liquid effects on organic reactions: getting the reaction outcomes you want¹ (in collaboration with Prof. Anna Croft, University of Nottingham; Dr Ron Haines and Dr James Hook, UNSW)

Ionic liquids are salts that melt below 100°C. They have potential as replacements for volatile organic solvents but outcomes of reactions in ionic liquids are often unexpectedly different to those in traditional molecular solvents. The focus of this project is to extend the understanding of ionic liquid solvent effects we have already developed and to use this knowledge to demonstrate that ionic liquids can be used to control reaction outcome. The project would involve using NMR spectroscopy to monitor reactions and kinetic analyses of these results, along with synthetic organic and analytical chemistry. The project can be readily tailored for students with more interest in the physical and analytical aspects, with the opportunity to develop new methods for following reaction progress and undertake molecular dynamics simulations, or to the more synthetic aspects, by focussing on designing new ionic liquids, increasing reaction yield and optimising isolation. That is, to get the reaction outcome you want!

b) Non-planar aromatic hydrocarbons: different reactivity based on structure² (in collaboration with Prof. Lawrence Scott, Boston College, USA)

Aromatic hydrocarbons are meant to be planar – right? Yet the synthesis of carbon nanotubes and related structures relies on the reactivity of curved aromatic systems. This project focuses on the different reactivities of these systems relative to 'normal' aromatics and how it might be controlled and exploited. It will predominantly involve synthesis and reactivity of systems, such as those shown below, with the opportunity for some kinetic studies to interpret the reactivity. Ultimately, understanding and exploiting these differences will allow the rational synthesis of these curved polyarenes.
c) Catalysis using N-heterocyclic carbenes: understanding structure/activity relationships

N-Heterocyclic carbenes, have significant roles in organo- and organometallic catalysis, however some carbenes are effective for some processes but not for others; the origin of this is not well understood. This project aims to relate structure and chemical properties of carbenes to catalytic efficacy, along with observing any solvent effects – this requires a series of chosen carbenes that vary in one way only (steric bulk, electronics, heteroatoms). Along with making the precursors to the carbenes, this project involves the opportunity to utilise various characterisation techniques and to undertake evaluation of catalytic systems; the latter can vary from simple screening of catalysts through to detailed kinetic analyses. The ultimate goal is to be able to rationally choose an NHC catalyst for a given process.

\[
\begin{align*}
\text{R} - \text{N} - \text{C} & \quad \text{involve sterics.}
\end{align*}
\]

\[
\begin{align*}
\text{R} - \text{N} - \text{C} & \quad \text{good solubility.}
\end{align*}
\]

\[
\begin{align*}
\text{R} - \text{N} - \text{C} & \quad \text{deteriorate solvation.}
\end{align*}
\]

d) Solvent-solute interactions in ionic liquids: can we design better solvents? (in collaboration with Dr Ron Haines, UNSW; Prof. Anna Croft, University of Nottingham; Dr Leigh Aldous, King’s College, & Prof. Bill Price, Western Sydney University)

We have previously made use of molecular dynamics simulations to understand interactions between a solute and the components of an ionic liquid; this can be used to explain why benzene is so soluble in ionic liquids and why certain reactions proceed faster on moving to ionic solvents. This project aims to extend this and to model - both with simple compounds and simulations – which ionic liquid would be better solvents for a given solute. In order to do this both physical measurements of solubility and molecular dynamics would be undertaken to highlight key solute-solvent interactions. The outcome would be a better understanding of what interactions are required to confer good solubility giving us the opportunity to ‘design’ appropriate properties into ionic liquids – and these could then be made!

For recent examples of our work in the above areas see:

We develop and apply methods of computational chemistry to elucidate the mechanisms underlying many processes in synthesis and in biochemical systems (http://www.chemistry.unsw.edu.au/hogroup). This enables us to design more effective chemical reagents, drug molecules or enzymes that our experimental colleagues can test or implement in practical applications. Topics of particular interest include, but are not limited to catalysis, solvent effects, supramolecular chemistry, and fundamental physical organic chemistry. We work closely with experimental groups, so projects can be tailored to include an experimental component. The following outlines several representative projects but feel free to come and chat about any other ideas you may have! No background in computational chemistry is assumed, and you will be equipped with valuable modelling skills at the end of your project.

(a) **Anionophores as novel anti-cancer agents**

Anionophores are molecules that bind anions, most commonly through hydrogen bonding. Recent studies have revealed that these molecules can also perturb the ionic gradient in cells by transporting anions across cell membranes thereby leading to cell death (see for example, *Nature Chemistry* 2017, 9, 667).

To further develop their potential as anti-cancer agents, we would like to simulate the transport process for several families of anionophores. In this project, you will learn how to carry out classical molecular dynamics simulations and build free energy profiles (fun stuff!). This project will help establish the molecular pre-requisites for anion transport, and facilitate the design of more effective drugs.

(b) **How important is reorganisation energy for binding guest molecules?**

Squaramides are an important class of molecules that are used in organocatalysis and anion receptor chemistry. The activity of these molecules is directly related to how tightly they bind guest molecules. For a long time, the acidities of the NH protons are used to gauge the strength of the hydrogen bonds they form with anions. However, our recent work (*J. Org. Chem.* 2017, 82, 10732) suggests that reorganisation energy, i.e. the energy required to transform the molecule into its active conformation, also plays a critical role. In this project, you will use very accurate quantum chemical methods to
delineate these contributions to the binding affinities of squaramides and related molecules. This work may also involve some synthesis and NMR experiments.

(c) Towards a Universal Approach for Solvation Modelling
In *ab initio* quantum chemistry, there is a well-known “variational principle” which provides a framework whereby gas phase energies can be systematically improved towards the “exact” result. However, such a theoretical framework does not currently exist for condensed phase simulations. Since much of chemistry occurs in the condensed phase, our group has a longstanding interest in developing robust computational procedures for calculating solution phase kinetics and thermodynamics (See for example: *J. Phys. Chem. B* 2016, 120, 1319). At present, approximate methods such as continuum solvation models that treat solvent molecules implicitly are the most popular because of their computational efficiency but they are valid only for specific solvents, and their errors are very large even for simple organic (e.g. S$_2$I$_2$) reactions. In this project, we would like to investigate the use of statistical theories and modern quantum mechanics and QM/MM force fields to develop more general and robust procedures for modelling solvation of elementary organic reactions.

(d) Quantum chemical modelling of nucleophilicity and basicity of N-heterocyclic carbenes

In this project, you will apply state-of-the-art quantum chemical methods to model structure-activity relationships of a powerful class of catalysts known as N-heterocyclic carbenes. The insights provided by computation will be used to guide the design of more effective catalysts, and there are opportunities to perform synthetic and characterisation studies to test your theoretical predictions.

(e) Computer-aided design of fluorinated bioactive molecules (with Dr. Luke Hunter)
This project will use computational techniques (e.g. docking, machine learning tools, QM and MD simulations) to determine the 3D shapes, logP values and protein-binding ability of a variety of fluorinated bioactive molecules. Examples of medicinally-relevant targets that are currently of interest within the Hunter group are shown below. There will also be an opportunity in this project to validate some of the computational predictions through synthesis.
FLUORINE IN MEDICINAL AND ORGANIC CHEMISTRY

- Fluorine is a small atom that packs a big punch. When incorporated into organic molecules, fluorine can have a dramatic impact on molecular properties such as $pK_a$, metabolic stability, 3D conformation, and binding affinity for protein targets.
- In the Hunter group, we are harnessing such effects to optimise the properties of a variety of bioactive molecules. We collaborate extensively to evaluate the biological properties of the fluorinated molecules that we create.

Here are some of the broad research areas within the Hunter group:

(a) Fine-tuning the shapes of cyclic peptides
Cyclic peptides are promising lead compounds for the treatment of a variety of diseases including cancer and malaria. However, there are two major limitations of cyclic peptides: (i) their synthesis via head-to-tail cyclisation is often inefficient; (ii) it is difficult to fine-tune the shapes of cyclic peptides to optimise their target binding. In this project, we are using fluorine chemistry to solve both of these problems. The key is to synthesise stereoselectively fluorinated amino acids, which are valuable shape-controlled building blocks.

Collaborators: Prof Maria Kavallaris, A/Prof Shelli McAlpine, A/Prof Renate Griffith, Dr Eddy Pasquier, Prof Vicky Avery

(b) Next-generation enzyme inhibitors
Aspartic proteases are enzymes that cleave other proteins in a sequence-specific manner. Aspartic proteases are involved in the life-cycles of several diseases including cancer, malaria and HIV, and thus they are potential drug targets. In this project, we are designing a new class of aspartic protease inhibitors. The key is to incorporate fluorine atoms into our inhibitors at very precise locations, in order to mimic the electron distribution of the activated intermediate of peptide hydrolysis.

Collaborators: A/Prof Renate Griffith, Dr Junming Ho
(c) **Towards a novel treatment for stroke**
Stroke is a leading cause of death and disability in Australia, and the treatment options are extremely limited. We are pursuing a new approach. We’re developing drugs that activate nerve cells’ natural hypoxia protective mechanisms (a kind of “high-altitude-chamber-in-a-pill”), which will put nerve cells into damage-control mode after a stroke. The key is a molecular-level understanding of the proteins that naturally activate this hypoxia response.

*Collaborator: Dr Nicole Jones, A/Prof Renate Griffith*

(d) **Editing the undesirable activity out of illegal drugs**
Gamma-Hydroxybutyrate (GHB) is a molecule with a bad reputation. It binds to neurotransmitter receptors in the brain, and it has previously been prescribed to treat a variety of ailments including alcoholism and depression. Unfortunately however, GHB also has sedative/hypnotic activity, which has led to its abuse as a “date-rape” drug. We believe that the bewildering variety of GHB’s effects can be attributed to the molecule’s conformational flexibility, which allows it to bind to many different neurotransmitter receptors. In this project, we are creating conformationally-restricted fluorinated analogues of GHB, in order to preserve the desirable activity while editing out the undesirable activity.

*Collaborator: Prof Mary Collins, Dr Junming Ho*

(e) **Molecular Velcro: creating new molecules that will stick to DNA and crosslink it in unprecedented ways**
Cancer is a common disease that kills 1 in 3 of us in the Western world. Chemotherapy is the principal treatment for metastatic cancer, but its effectiveness is limited by the resistance that tumour cells can develop to many conventional drugs. We are developing new drugs that will bind to DNA and weld the two strands together in a way that is difficult for tumour cells to repair. This will give potent anticancer activity, with a slower development of drug resistance.

*Collaborators: Dr Graham Ball, A/Prof Larry Wakelin*

All of the above projects (and others within the group) are based on synthetic organic chemistry as the major experimental technique. Other techniques that you might use include: molecular modelling; NMR; neuroprotection assays; solid-phase peptide synthesis; and DNA-binding biochemical assays.
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LASER PROBES OF CHEMICAL REACTIONS

- Use laser spectroscopy to characterise new free radicals;  
- Discover new chemical reaction mechanisms that cannot be explained by current theories;  
- Contribute to international atmospheric models to test hypothesized atmospheric processes;

It would be great to work with Honours students on the following projects:

(a)  Weird chemistry – reactions that just don’t go where they should. (Collaborators: Meredith Jordan, Sydney Univ.)

Since the 1930's, the concept of a transition state (TS) has formed the bedrock of chemical reaction theory. When the activation energy is very near the TS energy, the reaction becomes very slow and other unsuspected processes become competitive, even dominant. Over the past few years we have identified new chemical pathways never previously described.

The “Roaming” reaction: When a reaction is initiated near the energetic threshold, the products barely have enough energy to escape each other’s influence. Here, they “roam” around each other and re-collide, forming unexpected products. This project will seek roaming products from new photochemical reactions and to explore whether these new products play a role in the chemistry of the atmosphere.

(b)  Atmospheric Chemistry (Collaborators: Meredith Jordan, Sydney Univ; Dwayne Heard, Univ. of Leeds; David Osborn, Sandia Nat’l Labs, USA, Chris Hansen, UNSW)

Between 10^4 and 10^5 organic compounds have been measured in the atmosphere. This complexity makes developing a predictive atmospheric models very challenging. But such models are essential if we are to understand the role of chemical species on air quality, ozone depletion and climate change, and to predict the impact before releasing new compounds. Two projects are offered for 2019:

Dihydrogen (H2) in the atmosphere is a trace species with a concentration of around 500 parts per billion. As a long-lived species (half-life ~ 2 years), it has been considered to be relatively unimportant. However, atmospheric models cannot account for observed amount of H2. Modelers believe that there is a missing source of H2 that is photochemical in nature. The possibility that H2 will find broad application as a “green fuel” (there are already H2 cars) means that large-scale leakage of H2 into the atmosphere is likely. Mankind’s record of releasing compounds to the atmosphere, without understand the implications, has had severe consequences in the past (think about the ozone hole and global warming). We have the
opportunity to correct the weaknesses in atmospheric chemistry of H₂ before we reach this point. In recent research, we have discovered that many carbonyls are a source of H₂ when exposed to ultraviolet light. In this Honours project, you will make measurements of H₂ production from a series of aldehydes and work out the chemical mechanism and importance. Collaboration with atmospheric modelers is also a possibility.

The fate of fluorinated compounds (collaboration with Chris Hansen): Hydrofluorocarbons (HFCs) are effective alternatives to the chlorofluorocarbons (CFCs) and hydrochlorofluorocarbons (HCFCs) that have found widespread use in commercial products, but with no ozone depletion potential. However, HFCs have a different environmental drawback: they absorb infrared light very strongly, and have calculated atmospheric lifetimes ranging from decades to centuries. This leads to global warming potentials thousands of times greater than carbon dioxide (CO₂). These compounds began entering the atmosphere in the 1990s and will be there for centuries. Their atmospheric chemistry is not understood and more work is urgently needed to understand the pathways by which these species are removed from the atmosphere. This project can be tailored to have a significant computational chemistry component, or tailored to be almost exclusively experimental in nature, or anywhere in between.

(c) Radicals in the atmosphere and combustion (Collaborator: Tim Schmidt)

Free radicals are key intermediates in all complex chemical reactions. OH radical attack is the first step in the “processing” of nearly all atmospheric compounds. Processing can reduce the molecular weight, leading to fully oxidized products (CO₂ and H₂O) or increase the MW, reducing the volatility and leading to harmful aerosol formation. The processing of either biogenic emissions (e.g. terpenes) or anthropogenic emissions (e.g. toluenes) is largely unknown. There are several projects on offer for 2019, for example:

Radicals from OH attack on atmospheric species: OH can attack unsaturated hydrocarbons in two different ways: abstracting H to form H₂O and a radical, or adding across a π-bond to form an OH-adducted radical. The OH-adducted radicals have been scarcely measured in the literature. In this project you will investigate either a typical biogenic compound (e.g. α-pinene) or anthropogenic compound (e.g. cyclohexene) and react it with OH. The ensuing OH-adducted or abstracted radical will be isolated in vacuum and probed using laser spectroscopy to determine where the OH adds or attacks and the isomeric and electronic structure of the radical product. This will provide the first firm evidence for the assumed initial step in atmospheric processing of these compounds.

H-atom addition/loss from common fuels and biofuels: Hydrogen atoms can be lost from or gained by aromatic fuels, in both cases making radicals. In this project you will choose such a fuel, and use a custom-built reactor to make it gain or lose H. The resulting radical, the first intermediate in combustion, will be mass selected and probed by laser spectroscopy.

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BIOINSPIRED MATERIALS, TISSUE ENGINEERING, MECHANOCHEMISTRY

Inspired by biological materials, we integrate nano- and micro-fabrication techniques with synthetic chemistry to mimic the physical and chemical properties of the cell and tissue microenvironment. Much of our work is motivated by a dynamic model of the microenvironment where the interplay between chemical cues (extracellular matrix composition), physical cues (geometry, mechanics and topography) and biological cues (paracrine and juxtacrine signals) guides mechanochemical signalling to influence cellular identity, fate and function. Our broad aims are to:

1) Develop model synthetic platforms for cell biology research and high-throughput drug development.
2) Use the output from 1 to design clinically relevant biomaterials that direct a functional outcome (e.g. synthetic organoids, model tumours, tissue repair and replacement).

Our work is necessarily interdisciplinary; honours students will gain practical experience in synthetic chemistry, materials fabrication (bioprinting, lithography), and cell and molecular biology techniques.

It would be great to work with Honours students on the following projects:

(a) **Mechanochemical functionalisation of hydrogels** (w/ Prof. J. Kruzic, Mech. Eng.)

Hydrogels in tissue are viscoelastic materials that are continuously remodelled, and undergo dynamic changes in chemistry. Recreating dynamic chemistry in the laboratory most often involves incorporation of stimuli-responsive motifs, or secondary polymerization routines. We are investigating chemical linkages in hydrogels that are dynamic in response to stimuli including: temperature, pH, enzymatic activity and force. We are particularly interested in approaches where the chemistry can be modulated through applied compression or tension. Recently, we demonstrated how force-induced bond rupture in a disulfide linked poly(ethylene glycol) hydrogel facilitated reaction with an appropriate acceptor molecule within the material (Fig. 1; Mater. Horizons 2016). This approach is amenable to patterning virtually any molecule with the appropriate conjugation tag, and represents a new route to modifying the mechanics and chemistry of soft materials. There are several other dynamic linkages that we are interested in investigating.

(b) **Directing the chemistry/architecture of 3D extruded soft biomaterials** (w/ Prof. J. Gooding)

3D printing of cells and tissues is limited by issues with complex bioink formulation, segregation of different cell types, cell viability during prolonged printing, and difficulty recreating complex architectures observed in nature. New methodologies to quickly fabricate cell-laden...
tissue structures with well-defined segregated populations has the potential to be transformational to tissue engineering. We are exploring the extrusion of multiple hydrogel materials of tissue-mimetic composition (Fig. 2; Advanced Materials 2015). By incorporating chemical handles in the polymers, microfluidics will be employed to establish gradients of multiple cell binding ligands. We aim to develop co-culture formulations for translation to a 3D printer to direct write the cell-laden extruded hydrogels within a 3D bulk poly(ethylene glycol) hydrogel.

(c) Magnetoactive hydrogels to drive cell and tissue engineering

Cells in vivo interact with matrices that are dynamic, with many physiological and pathological processes governed by changing mechanics and matrix presentation. However, recreating these microenvironments in the laboratory has proved challenging. We have developed a composite magnetoactive material—where stiffness can be reversibly modulated across the full spectrum of physiologically relevant mechanics—to study temporal relationships in cell-matrix interactions. Enabled by the dynamic reversibility, we discovered critical time periods during osteogenesis where stiffening guides lineage specification (Fig. 3; Adv. Health. Mater. 2016). These materials can be adapted to multiple hydrogel systems, and use simple permanent magnets, which will broaden the use of this technique to virtually any laboratory. New directions in this project involve: 1) the investigation of stiffening and softening in hydrogel materials with reversible bonds (e.g. H-bonding in polysaccharides), 2) covalent tethering of iron oxide nanoparticles within the hydrogel framework, and 3) establishing a 3D magnetoactive tumour microenvironment for therapeutic development.

(d) Synthetic tumours for cancer nanomedicine development (w/ Prof. M. Stenzel)

Our interests in cellular “plasticity” has led us to cancer, where we believe progression and metastasis is a consequence of dynamic interactions in the tumour microenvironment that promote intravasation, extravasation and colonization. We microengineered small populations of melanoma cells across hydrogels and were able to uncover an intriguing role for geometry at the perimeter of these micro-tumors in orchestrating the activation of a cancer stem cell (CSC) state (Figure 4; Nature Materials 2016). This is important because these CSC-like cells are believed to be the root cause of recurrence and metastasis, the primary causes of suffering in cancer. Our vision for the future of this work is the integration of our model systems into autonomous tissue-mimetic architectures, for therapeutic development on patient derived cells. We have several new directions in need of students including: new hydrogel chemistry and fabrication techniques, exploring spatiotemporal uptake of nanoparticles, integration of multiple different cell types.


Climate changes, depletion of fossil fuels, and global warming have encouraged scientific society to consider utilising energy from sustainable resources, including wind power and solar energy. Despite the fact that sustainable energy sources are highly abundant, the supply of sustainable resources fluctuates all the time.¹ ² Recent advances in lithium-ion battery technology have enabled a power source ranging from portable electronic devices to electric vehicles. In the future, developing energy storage applications for renewable resources will become increasingly important.³

I am opening a new research group which focuses on developing next-generation energy storage system. Our research project will combine synthetic chemistry, electrochemistry, and materials science principles to develop advanced energy storage devices, in particular, rechargeable batteries. We are expecting to conduct interdisciplinary research and establish collaborations with other research groups.

Please feel free to contact me if you need any further information.

It would be great to work with Honours students on the following projects:

(a) Rechargeable Al-ion Batteries – (In collaboration with Prof. J. Fraser Stoddart at Northwestern University)

Aluminium is the third most abundant element in the Earth’s crust. (ref) It has one of the highest theoretical volumetric capacity (8056 mAh mL⁻³) on account of its multiple redox states.⁴ Therefore, developing rechargeable batteries utilising aluminium offers a golden opportunity for delivering a high energy to cost per price.⁴ The development of Al-ion batteries has not reached a stage yet. It has proved difficult to design an electrode material that can reversibly intercalate Al-ions, because the multivalent nature of aluminium is accompanied by significant structural changes, resulting in a rapid capacity fading.

Based on preliminary and unpublished results, we envision that redox-active compounds could undergo reversible Al-ion intercalation through electrochemical processes. The overarching goal of this program is unlocking the full potential of rechargeable Al-ion batteries, by combining synthetic organic chemistry and battery engineering. Based on the large selection and synthetic versatility of various organic
molecules\textsuperscript{5}, the redox-active compounds based rechargeable Al-ion batteries could provide a promising starting point for developing affordable large-scale energy storage applications.

Figure 1. (a) Theoretical volumetric and specific capacity of Li-ion and Al-ion batteries. (b) Battery cell comparison between Li-ion and Al-ion batteries. (c) Electrochemical redox of quinone-based macrocyclic compound. Upon discharging, the macrocycle is reduced to its semiquinone state. Followed by interacting with the cationic chloroaluminates, which were generated by the asymmetric cleavage of dialuminium hexachloride, resulting in the formation of tetracoordinated aluminium complex.

(b) Lithium Sulphur Battery – (In collaboration with Prof. Do Kyung Kim at KAIST)

The Lithium–Sulphur system is a promising high-performance battery candidate for large-scale application on account of its high theoretical specific capacity.\textsuperscript{6} However, it has come up short on delivering long cycle life mainly due to the formation of soluble polysulphides\textsuperscript{3}, which results in the loss of active material during redox processes. In this project, we will design a 1-dimensional hollow nanostructure electrode as well as encapsulates sulphur within the electrode, in order to prevent the dissolution of polysulphides throughout the battery cycling process.

\begin{tabular}{|c|c|c|c|}
\hline
Anode & Electrolyte & Cathode \\
\hline
Lithium-ion Battery & Graphite & Organic solvent & Inorganic compounds \\
\hline
Aluminium-ion Battery & Aluminium & Ionic liquid & Redox-active compounds \\
\hline
\end{tabular}

\begin{tabular}{c}
\textbf{Rechargeable} \\
\textbf{Aluminium-ion Batteries} \\
\textbf{Based on} \\
\textbf{Redox-active Compounds} \\
\end{tabular}

SYNTHETIC ORGANIC AND MEDICINAL CHEMISTRY

The main focus of the research undertaken in my group is the discovery and development of novel bioactive molecules. Naturally produced chemicals are of fundamental importance in biological systems. Such chemicals are used to mediate interactions across all levels of biological hierarchy. Very often such diverse molecules are produced only in minute quantities. New or innovative organic syntheses not only provide access to sufficient quantities of these molecules but also their analogues. The access to various structurally-related analogues allows full assessment of their biological activity and mode of action, and offers opportunities to develop new therapeutic leads. The research is multi-disciplinary in nature and involves a combination of synthetic organic chemistry, molecular modelling and biological screening.

(a) **DESIGN AND SYNTHESIS OF NOVEL ANTIMICROBIAL AGENTS**

*Quorum Sensing Inhibitors*

The emergence of multi-drug resistance in common human pathogens has highlighted the need to develop novel classes of antimicrobials for the treatment of human disease. A number of projects are available in this area focussing on a combination of organic synthesis, molecular modelling, and *in vitro* and *in vivo* antimicrobial screening. This project will develop novel antagonists of bacterial signalling pathways, which inhibit the regulatory quorum sensing communication pathways of bacteria, and will model the receptor-ligand interaction using the X-ray crystal structures of bacterial signal receptors e.g. AHL receptor LasR. This represents a non-growth inhibition strategy that is less likely to result in the development of drug resistance. In particular, this proposal will investigate the design and synthesis of a range of novel heterocyclic compounds with antimicrobial activity.

*New scaffolds for antimicrobial discovery*  
(in collaboration with Prof. David StC Black)

The majority of conventional antibiotics used today share a common feature in that they act on specific molecular targets. Having very well-defined targets, these drugs act with a high degree of selectivity, minimizing unwanted side effects. However, a major limitation of antibiotics targeting a single receptor is the ease with which resistance can be developed. The central aim of this project is to design novel small molecular antimicrobial peptide (SMAMP) mimics based on biphenyl scaffolds, which disrupt the normal functioning of the membranes of the bacterial cell, and
as a consequence allow the development of antimicrobial agents with enhanced activity and the ability to bypass resistance mechanisms used by bacteria against other antibiotic types.

Small Antimicrobial Peptides
(In collaboration with Dr Adam Martin)
The rapid emergence of bacterial resistance to current antibiotics further increases the need for development of alternative anti-infective strategies. Antimicrobial peptides (AMPs) are a diverse array of naturally-occurring molecules that possess bactericidal properties. AMPs act via non-receptor interactions. Their mechanism of action is predominantly attributed to their facially amphiphilic structure. This project aims to synthesize a series of small AMPs and elucidate their mechanisms of action using a variety of techniques including supported lipid bilayers (IBLM), atomic force microscopy and fluorescence microscopy. Small amphiphilic short peptides are remarkably versatile materials which can self-assemble into a variety of elegant structures. Functionalisation of the N-terminus of these short peptides with aromatic groups can result in self-assembly into hydrogels composed of long, entwined fibres. The modified peptides would be studied for their localisation and/or transportation across the bacterial cell membrane.

(b) DEVELOPING ANTICANCER COMPOUNDS THAT ACTIVATE GLUCOSE OXIDATION
(in collaboration with Dr Kyle Hoehn, BABS, UNSW)
Cancer is a major burden of disease, affecting the lives of tens of millions on a global scale. A hallmark feature of nearly all cancer cells is their altered metabolism of glucose compared to non-cancerous cells. Relative to most normal cells, cancer cells use a greater proportion of incoming glucose for non-oxidative purposes including the production of building blocks for cell division (lipid, DNA and protein), rather than oxidative pathways that produce carbon dioxide (CO₂) in mitochondria. The goal of this proposal is to develop anticancer molecules that change cancer cell glucose metabolism to be more like that of non-cancerous cells. We have identified a small molecule that increases glucose oxidation and selectively kills cancer cells in vitro and in mice. The aim of this project is to generate new derivatives with enhanced activity and drug-like properties. The new compounds will be evaluated for anticancer activity in various cancer cell lines.

(c) NOVEL CYTOSINE ANALOGUES AS ANTI-CANCER AGENTS
(in collaboration with Dr Ashwin Unnikrishnan)
Myelodysplastic syndrome (MDS) is a group of cancer diseases that affects normal blood cell production in the bone marrow. Patients diagnosed with MDS often die as a consequence of bone marrow failure and progression to acute myeloid leukaemia. Currently, the front-line treatment of such disease is the cytosine analogue, 5-azacytidine (AZA), which acts as a DNA methyltransferase (DNMT) inhibitor that reduce tumour formation in part through the increase expression of tumour suppressor genes. However, the use of the currently developed inhibitors has been limited by their high cytotoxicity, as well as their poor bioavailability and stability in physiological environments. The aim of this project is to generate a variety of new cytosine derivatives with enhanced activity and drug-like properties. The new compounds will be evaluated for anticancer activity in various cancer cell lines, and their mechanism of action.
Educators have progressed significantly in the past 50 years in understanding how students learn, specifically in chemistry [1-3], however there is still much to discover, develop and implement into our teaching to provide an outstanding educational experience at UNSW. We hope to address the unique difficulties students learning chemistry encounter using modern technologies backed by evidence-based research.

Are you interested in doing research in chemical education? Do you aspire to make an impactful difference on the way we educate our students? The following projects may be just right for you:

(a) Effects of threshold/mastery learning
As part of the exciting new changes to first year chemistry a novel assessment method is being used, expanding on similar changes made to the award-winning undergraduate laboratory program that tested laboratory skills. In this novel assessment students must show complete knowledge of threshold concepts by completing hurdle tasks and online lessons to receive a pass in the course.

You will have the opportunity to engage with this exciting and innovative project by focussing on the following research questions that may influence future directions of undergraduate teaching:

- Do students study differently for threshold assessments compared to traditional models?
- Are students more effective at recalling and applying the threshold knowledge?
- Does this assessment model lead to better understanding of threshold concepts?
- Is the blended (online and face-to-face) material more helpful for novice students?

(b) Development of online chemistry activities
Technology has expanded the possibilities of where teaching can go. When used effectively it can greatly aid in learning and increase efficiencies in teaching [4]. Game-based apps provide an entertaining way to learn potentially boring or repetitive content. Some apps specifically for chemistry already exist [5] but are not yet integrated into the curriculum at UNSW. If you are interested in developing gamification aspects and game-based apps and researching their impact on student’s learning in Chemistry then you could be involved in some exciting projects in this field.
(c) Have your own idea(s)?

If you have your own idea for a project that aligns with our philosophy then we would like to hear from you. Get in contact with me and we can discuss your project idea(s).

References

CHEMISTRY EDUCATION IN THE 21ST CENTURY

The UNSW chemical education group is interested in improving the learning outcomes and experience of Chemistry students and contributing to the chemical education research community. My personal research interests encompass how to integrate the global challenges facing science into chemistry curricula (systems thinking), the development and tracking of transferable skills of chemistry graduates and the role that technology must play on how we teach and interact with chemistry. Here are some of the projects available for honours/research project with me, though chemical education projects can be tailored and developed to suit you and your interests!

(a) Facing up to global challenges - Integrating systems thinking into Chemistry education

Keywords: Systems thinking, Global challenges, Mastery learning

The world is currently facing unprecedented challenges which are affecting all facets of life on earth. Climate change, Sustainability and the need for Renewable energy sources and storage are challenges which have chemistry at their core. A recent article in Nature Reviews Chemistry¹ served as a call to arms for chemistry educators to integrate systems thinking into chemistry curricula at all levels to empower our students with the knowledge and skills to face these challenges. Systems thinking is about putting chemical concepts into a real worlds context and showing how atoms and molecules (and the decisions we make with what to do with them) impact people’s lives and our environment. There is very litter literature which describes systems thinking in chemistry which presents many exciting opportunities for your project from exploring the challenges of integrating it into chemistry curricula to finding out how student’s viewpoints develop and change with a broader view of chemistry…it’s an exciting time to be alive!

(b) UNSW Chemistry Graduates: Ready for Anything... But do they know that?

Keywords: Transferable skills, Work Integrated Learning, Micro-credentialing

Beyond an understanding of key concepts of chemical theory, Chemistry graduates require a unique set of transferable skills. UNSW Chemistry has recently introduced several exciting education developments designed to enhance the capabilities and skills of our graduates. We are interested in investigating the efficacy of these programs in the development of transferable skills as well as exploring how well our graduates can articulate their skills in a chemistry context (such as when applying for jobs or networking) and how we might develop an educational intervention to improve this.

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(c) There's an app for that! Pedagogical content knowledge in the age of technology

Keywords: Digital Literacy, PCK, TPACK, Online learning, Blended Learning

Pedagogical content knowledge (PCK) theory recognizes that beyond the teacher’s own understanding and knowledge of the content theory there is a surrounding body of knowledge to do with how students learn and process information specific to the theory being taught. In the age of technology, the way we interact with students has changed. Technological pedagogical content knowledge (TPACK) is the basis of effective teaching with technology, requiring an understanding of the representation of concepts using technologies; pedagogical techniques that use technologies in constructive ways to teach content; knowledge of what makes concepts difficult or easy to learn and how technology can help students overcome difficulties. How students engage with technology to learn is rapidly evolving. Like many other institutions, online learning is now one of our underpinning methods of teaching first year chemistry. What is not well understood is what strategies students are engaging to use and supplementing these materials to facilitate learning. Why are some formats preferred by students and how is this impacted by demographics? Is there potential to impact how effectively we can teach students chemistry by ‘updating’ our TPACK?

(d) Research by Students: Developing an innovative program that facilitates high volume contributions to a newly designed urgently needed online spectroscopic database (collaboration with Laura McKemmish).

Keywords: Spectroscopy, Django online Python databases, Citizen Science, Education/Outreach

This project has a bit of everything: programming, data science, spectroscopy and education.

This project enables high school and undergraduate students to contribute to an urgently needed online database, gaining valuable transferable skills, scientific knowledge and exposure to scientists and scientific research in a project linking research, teaching and outreach!

The Database: Update of 1979 Huber & Herzberg Constants of Diatomic Molecules, still cited once a day, into a modern online query-able database. This data is exceptionally useful in benchmarking quantum chemistry and predicting spectra for diatomics found across the universe for applications from monitoring to detection to creating the coldest molecules ever!

The Education Component: This ‘research-in-schools’ approach is part of a growing international movement including the US SEED program championed by UNSW staff member and Nobel Laureate Sir Fraser Stoddard. Here, we will investigate how to bring it to Australia, probably through the new “Science Extension” HSC course, through a thorough study of related approaches and interviews of high school teachers.

SYNTHETIC ORGANIC AND MEDICINAL CHEMISTRY

- Synthesis: develop new anticancer molecules that target heat shock proteins
- Biology: understand the role that heat shock proteins play in cancer cell growth
- Medicinal Chemistry: identify the mechanism of action of new structures

We have the following projects available for Honours students:

(a) Developing new molecules that target cancer: heat shock protein 70 (Hsp70) inhibitors

A molecule that can selectively kill cancer cells and not impact normal cells would be of tremendous therapeutic interest. Targeting a protein involved in rapid cell division is an approach likely to achieve this selectivity. One such protein, heat shock protein 70 (Hsp70), controls protein folding events that are required for rapid cell division. Molecules that could control Hsp70’s role in protein folding would provide fundamental new knowledge about critical protein folding processes, which may lead to new discoveries for selectively targeting cancer cells. In this project you would learn how to synthesize molecules utilizing solution and solid phase chemistry. You will learn how to run proton and 2-D NMR, LCMS, and column chromatography. You will also have the opportunity to learn how biological assays work on your compounds, including cell death, cell permeability, protein level analysis via western blots, protein folding assays, and protein expression.

(b) Build molecules that controls protein folding and disease

Many diseases are the result of an imbalance between proteins being produced, folded, and degraded. Alzheimer’s and Parkinson’s result from improperly folded or aggregate proteins; facilitating the folding of aggregates may successfully treat these diseases. Cancer relies on cells to be highly efficient at folding proteins; inhibiting the folding process may successfully treat malignancy. Heat shock protein 27 (Hsp27), a small chaperone, initiates protein-folding events and its inadequate or excessive function is connected to diseases such as Alzheimer’s and cancer respectively. Developing a molecule that controls Hsp27’s function by switching protein folding on or off would afford fundamental new knowledge about critical protein folding processes and shed light on these diseases. In this project you
would learn how to synthesize molecules, and multiple techniques including how to run reactions in solution and on solid phase. In this project you would learn how to synthesize molecules utilizing solution and solid phase chemistry. You will learn how to run proton and 2-D NMR, LCMS, and column chromatography. You will also have the opportunity to learn how biological assays work on your compounds, including cell death, cell permeability, protein level analysis via western blots, protein folding assays, and protein expression.

(c) Developing prodrugs: a general approach for building cell permeable drug molecules

This project will involve the synthesis of prodrugs that can enter cells and where masking groups are cleaved in cell lysate revealing the active molecule. The approach for this project will involve the incorporation of masking polar side chains with methyl groups, which are easily removed upon cell entry via enzymes. Prodrugs will also incorporate N-methyls on the backbone amide bonds and D-amino acids, both modifications disrupt intramolecular hydrogen bonds within a macrocycle and change the orientation of the side chains in such a way as to improve cell permeability. The prodrug molecules will also include asparagines, where these side chain amides increase transport across the cell membrane. In this project you would learn how to synthesize molecules utilizing solution and solid phase chemistry. You will learn how to run proton and 2-D NMR, LCMS, and column chromatography. You will also have the opportunity to learn how biological assays work on your compounds, including cell death, cell permeability, protein level analysis via western blots, protein folding assays, and protein expression.
Want to do research on a computer not in a lab? Love spectroscopy, quantum mechanics and energy levels? Feel constantly pulled between physics and chemistry? Or perhaps you want to utilise and strengthen your maths, programming and/or data science skills by exploring exciting molecular science applications from interpreting NMR spectroscopy to helping find aliens on exoplanets?

I am looking for keen students to undertake Honours projects with customisable amounts of chemistry, physics, mathematics, programming, data science and education/outreach. During an Honours project with me, you can expect to develop and strengthen many key transferable and scientific skills such as Python, command line, power use of supercomputers/ computer clusters, power use of quantum chemistry software packages, data science, data presentation, computational debugging and, perhaps most importantly, “Googling”.

Some of the projects available for this year with me include:

(a) Elucidating the structural-spectral relation for complex NMR spectra of peptides using computational chemistry with specialised and novel basis sets (collaborations with Shelli McAlpine and Luke Hunter).

**Keywords:** Computational Chemistry, Link with Experiment, Basis Set Design, NMR spectroscopy

NMR is a ubiquitous technique extensively utilised throughout the sciences, but most especially by the synthetic chemistry community. There are two issues associated with NMR spectroscopy: assigning the spectra accurately, and understanding what the assigned spectra tells us about the structure of the molecule. Accurate computational chemistry calculations can assist with both these tasks for difficult cases like fluorine-containing compounds and macrocyclic peptides. However, existing calculations often use sub-optimal basis sets that do not adequately describe the electron core region (See figure), with scaling factors used to fix these inadequacies.

This project has two main aims: (1) assessing the effectiveness of different basis set choices in understanding NMR spectra of fluoro-containing compounds and macrocyclic peptides, including potentially the use of novel ramp-Gaussian basis sets, and (2) use calculations to interpret experimental NMR spectra to determine molecular conformations.
(b) High volume prediction of approximation spectra for exoplanet characterisation (collaboration with Clara Sousa-Silva, MIT).

**Keywords:** Computational Chemistry, Astronomy, Exoplanets, Spectroscopy, Python, Supercomputers

Amazingly, astronomers can now not only detect exoplanets, they now have tools to identify molecules within their atmospheres using spectroscopy: eventually, this technology is expected to provide the best evidence for the presence or absence of alien life! However, even with new telescopes, the resolution and spectral coverall can be quite low, which means it is possible to misidentify molecules if their spectra are similar. In this project, we are looking at predicting approximation spectra for 14,000 small molecules that have been identified as stable and potentially volatile and thus viable biosignature gases (Astrobiology, 2016, 16, 465).

(c) Research by Students: Developing an innovative program that facilitates high volume contributions to a newly designed urgently needed online spectroscopic database (collaboration with Shannan Maisey).

**Keywords:** Spectroscopy, Django online Python databases, Citizen Science, Education/Outreach

This project has a bit of everything: programming, data science, spectroscopy and education. This project enables high school and undergraduate students to contribute to an urgently needed online database, gaining valuable transferable skills, scientific knowledge and exposure to scientists and scientific research in a project linking research, teaching and outreach!

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**The Education Component:** This ‘research-in-schools’ approach is part of a growing international movement including the US SEED program championed by UNSW staff member and Nobel Laureate Sir Fraser Stoddard. Here, we will investigate how to bring it to Australia, probably through the new “Science Extension” HSC course, through a thorough study of related approaches and interviews of high school teachers.
SYNTHETIC AND MEDICINAL CHEMISTRY

- Natural products deliver novel leads for pharmaceuticals in a diverse array of therapeutic areas and offer an excellent starting point for medicinal chemistry programs. A major focus of Prof Morris’s research interests are on the development of natural products as biomedical agents.
- Being able to synthesise new molecules in an efficient manner is critical and as such, the focus is on developing strategies to prepare these valuable materials and generate analogs that have improved potency and selectivity.
- The expertise gained from working on these areas leads to a number of collaborations with biomedical researchers where students can become involved in the understanding the biology.

It would be great to work with Honours students on the following projects:

(a) **Total Synthesis of Biologically Active Natural Products**
The development of efficient syntheses of biologically active natural products continues to be a major activity of the Morris group, with recent targets including ancirotzanazine A, embellistatin and coproverdine. As syntheses of these targets are completed, work is initiated on their mode of action and their suitability as therapeutic agents. Total synthesis is one of chemistry’s most exciting and challenging dimensions, providing you with excellent and broad training in synthetic chemistry. It will develop and hone skills in planning, retrosynthetic analysis, determining mechanisms, and structure elucidation.

(b) **Developing Inhibitors of RNA Splicing Kinases**
The control of the fundamental biological process of alternative splicing is an emerging method for treating diseases such as aged macular degeneration and cancer. It has been established that by controlling the phosphorylation of key proteins in the spliceosome it is possible to switch alternative splicing and generate particular protein isoforms.

The Morris group is actively engaged in the development of small molecules that can do this, and this is achieved by targeting the protein kinases that
mediate the phosphorylation. This work originated from earlier work on the synthesis of a natural product. Variolin B is a member of a unique class of marine alkaloids isolated from an extremely rare Antarctic sponge. It is no longer available from its natural source. The Morris group have devised a synthesis of variolin B that has restored access to the material and allowed further biological studies to be carried out. From this work it has been established that variolin B is a potent kinase inhibitor and represents an important scaffold for the development of kinase inhibitors. A range of analogs have been developed that are more selective inhibitors of certain kinases, as well as have better properties (such as solubility).

Our recent publication (*ACS Chem. Biol.*, 2017, 12, 825) describes how we have developed a new class of kinases inhibitor that selectively inhibits the kinase SRPK1 and has led to the identification of a series of molecules that are currently being developed as a treatment for aged macular degeneration, in collaboration with Exonate.

The Morris group is focused on developing selective inhibitors of the various RNA slicing kinases (the CLKs, DYRKs and SRPKs), with appropriate drug-like properties so they can be used as chemical probes to help understand the role these important kinases have on biological systems. A combination of synthesis and structure-based drug design is used to do this work, with students able to use Schrodinger and Cresset software to aid their design work.

(c) Developing the AAL(S) Scaffold for Therapeutic Applications (collaborations with Assoc Prof Nigel Turner (SOMS), Prof Alaina Ammitt (UTS), Dr Nikki Verrills/Dr Matt Dun (Newcastle)

Ceramide synthase (CerS) and protein phosphatase 2A (PP2A) are two enzymes that play a critical role in the regulation of multiple cellular signalling processes. The malfunctioning of these two enzymes has been found to have implications in diseases such as cancer, diabetes, asthma and neurological diseases including Alzheimer’s disease and stroke. Little is known about the biological mechanism of these enzymes and in particular, how they cause such diseases. To gain insight into these biological processes, the CerS and PP2A binders, FTY720 and AAL(S), will be used to explore the binding site of both enzymes and allow the identification of chemical probes which can be used to develop an understanding of the biological mechanisms of these complex diseases.

Development of the AAL(S) scaffold will allow for analog production which along with key biological testing will provide key information towards revealing the biochemical pathways and proteins involved regulating both enzymes at a molecular level. With Prof Ammitt, work is focused on using these molecules for the development of therapeutics for the treatment of asthma, whereas with Asoc Prof Turner we are developing molecules to elucidate the role of CerS in fat metabolism (see Turner et al, *Nature Communications*, 2018, 9: 3165 | DOI: 10.1038/s41467-018-05613-7)
Our research focuses on exploiting the flexibility of coordination chemistry to explore and develop molecular switching properties in polymeric metal-organic complexes. We focus on a type of molecular switching process called ‘spin crossover’ where two distinct electronic states can be accessed by temperature or pressure variation and light-irradiation. This fascinating process is accompanied by distinct changes in structure, colour and magnetic signal with potential application in data storage, display and sensing industries.

Skills you will learn:

- Organic and inorganic synthetic chemistry
- Making beautiful crystals!
- Structure elucidation (X-ray and electron diffraction / Australian Synchrotron / ANSTO)
- Magnetic, spectroscopic and calorimetric measurements and analysis

It would be great to work with Honours students on the following projects:

(a) Functional coordination polymers

Coordination polymers are constructed by bridging metal ions with organic ligands and have uses in a vast range of materials science applications. In this project, we will target metal ions capable of molecular switching and use temperature, pressure and light-irradiation to entice switching between electronic states. With the help of single crystal structural analysis, magnetic measurements and spectroscopy, we will uncover structure-function relationships and new functional coordination polymers.
(b) **Switchable square and cage complexes**

Molecular squares and cages are constructed by the molecular building block approach (“molecular lego”). In this project we use pre-designed building blocks (metals and ligands) to form, for example, dinuclear, square and cage complexes. The focus will be on including d⁶⁻⁷ transition metal ions which can be converted between high and low spin states by temperature, pressure and light-irradiation and investigate switching properties in both solution and solid state (aka beautiful crystals!).

![Switchable square and cage complexes](image)

(c) **Molecular switching nanocrystals**

Nano-sized crystals of inorganic materials can be prepared by a range of techniques. This project focuses on preparing “small” crystals of coordination polymers and discrete molecules which show molecular switching properties. The overall properties of such materials are extremely sensitive to sample quality, so we will explore the use of microfluidic techniques to prepare nanocrystals that are highly crystalline and contain minimal defects. In this project you will gain skills in a range of X-ray and electron diffraction techniques and various magnetic and spectroscopic methods.

![Molecular switching nanocrystals](image)
Nguyen’s group has several Honours projects focusing on the development of novel organocatalytic systems or unusual molecules and applications of those in synthetic organic chemistry.

(a) Project NTV1 - Tropylium Ion as Chromophore for Organic Dyes
Tropylium ion is an unusual non-benzenoid aromatic system with 6π-electron 7-carbon-ring structure.[1] Recent synthetic advances by our group have made this unique species much more accessible and understood, allowing us now to start to utilize it for a wide range of applications in organocatalytic chemistry[2-5] and photochemistry. This project will further investigate our recent findings that tropylium can be used as a versatile chromophore for a family of very interesting organic dyes and luminescent materials for metal and pH sensing. As some aspects of this project are confidential, students are encouraged to discuss with Vinh in person about this project.

(b) Project NTV2 - N-Heterocyclic Olefins as Novel Organocatalysts
Recently, N-Heterocyclic Olefins (NHOs, see scheme) have emerged as a new class of valuable reaction promoters with interesting action mechanisms. These compounds can be conveniently produced from commercially available precursors in one step. NHOs were originally targeted as a series of active agrochemicals in the 1970s, but they slowly revealed to be a far more interesting
compound family. Due to the donating ability of the two nitrogen atoms, the exocyclic C-C double bond is very electron-rich and strongly polarized. This interesting feature of NHOs offers multinucleophilic reactivity over the ketene aminal frameworks. Due to the strong nucleophilicity of the $\alpha$-carbon, NHOs can act as strong Lewis/Bronsted bases. This project will focus on synthesizing a family of NHOs, estimating their basicity and applying them as organocatalysts to promote environmentally friendly chemical processes. Students are encouraged to discuss with Vinh in person about this project.

(c) Project NTV3 - Tropylium-Based Host-Guest (collaboration with A/Prof Pall Thordarson)

This project will explore the potential of tropylium-bearing systems in host-guest chemistry in collaboration with A/Prof Pall Thordarson’s group. The electron-deficient nature of tropylium moiety makes it particularly attractive for the binding and sensing of small and medium-sized biologically important anions such as chloride, phosphate and carbonates. We propose the synthesis of tropylium-based macrocycles (see figure) as the starting point for this project, which will represent a new platform in supramolecular chemistry. Please also see Thordarson’s Honours projects for more details.

References
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HIGH-THROUGHPUT MASS SPECTROMETRY, ION-MOBILITY, STRUCTURAL CHEMISTRY AND CATALYSIS

- Robotic analysis of dynamic combinatorial solutions; screening of large chemical data sets
- Development of advanced ion-mobility MS-based analyses to probe self-assembly
- Determining structure-activity relationships related to self-assembly & catalysis
- Accurately calculating electronic structure, topology and energetics of molecules & assemblies
- Direct future synthesis towards more efficient processes; assess activity & function

Research Interests
Understanding the intrinsic properties of molecules, molecular building blocks and aggregates is key to realizing the bottom-up design of functional molecules and materials, and catalysts. We explore such molecular units in isolation, for example, via the pristine gas phase environment of specially modified mass spectrometers. The end goal of this research is the rational design of efficient catalyst and enzyme-like molecules.

The significant industrial potential of self-assembly to fabricate highly functional materials is hampered by a lack of knowledge of critical reaction intermediates, mechanisms and kinetics. Our group’s research addresses this knowledge gap by developing methods to (1) directly observe the molecular evolution of model self-assembly reactions with high temporal and structural resolution and (2) interrogate the intrinsic gas phase functionality of the assemblies themselves, including aggregation, inclusion and disassembly behaviours. This will determine the critical link between the assemblies’ structure and function, and provide the rational framework needed for optimising and directing synthetic outcomes.

Mass spectrometry as a probe for molecular self-assembly
Electrospray ionization-mass spectrometry (ESI-MS) is an effective technique for characterising reaction intermediates in synthetic and catalytic transformations. Additionally, ion-mobility spectrometry (IMS) has emerged as a very powerful technique for monitoring self-assembly. IMS is ideal for examining the size and shape of non-covalent complexes. It offers the advantage of isomer separation on the millisecond timescale, and measurement of the assembly’s topology, and as such, enables the study of conformational dynamics within that time frame. Together ESI-MS and IMS represent two complementary analytical methods of monitoring reaction solutions on a millisecond timescale.
Unique techniques used in the group include:
- advanced mass spectrometry and ion-mobility mass spectrometry,
- robotic analysis of dynamic combinatorial solutions, with screening of large chemical data sets,
- electronic structure and trajectory methods of computation for structure and function,
along with a variety of kinetic, wet chemistry and chemical characterisation techniques.

Projects and collaborations include:
- Assembly and reactivity of n-confused porphyrins (P. Weis, KIT)
- Dynamic combinatorial solutions and self-assembly of bis-β-diketonates (J. Clegg, UQ)
- Unusual complexation behaviours of cyclotricatechylene clusters (B. Abrahams, UoM)
- Encapsulation of ions by cyclophanes in solution (T. Brotin, ENS Lyon)
- Effect of fluorine on catalytic and metal mediated reactions
- Development of ion mobility and mass spectrometric techniques for analysis of reaction intermediates in solution (W. A. Donald, UNSW)

Potential students are highly encouraged to discuss their research interests with Dr Rijs.
We are interested in design, synthesis and characterisation of biomaterials and developing surface modification techniques for tissue engineering and regenerative medicine with an emphasis on clinical translation.

(a) Development of a technology for 3D printing of porous bioactive ceramics for treatment of hard tissue defects without using sintering; ink optimisation

Repairing large bone defects remains a major surgical challenge and suboptimal outcomes can have significant socio-economic repercussions and negatively affect quality of life. The aim of this project is to develop a 3D printing process to fabricate a custom-design synthetic bone graft. Currently, there are various 3D printing techniques for fabrication of ceramic scaffolds. However, these scaffolds need high-temperature sintering after printing that makes it impossible for incorporation of biomolecules such as growth factors and drugs.

(b) Nanocomposite cardiac patches for treatment of myocardial infarction

Cardiovascular diseases are the leading cause of death globally. In case of myocardial infarction, the regeneration ability of damaged heart tissue is severely limited. Tissue engineering offers promising strategies for cardiac regeneration, by combining biomaterials and cardiomyocytes. The aim of this project is to fabricate a tissue engineered patch that provides optimal structure, mechanical strength, and bioactivity for cells that can stimulate formation of new vasculature, and facilitate oxygen and nutrient transfer to the damaged region.

(c) Synthesis of porous calcium phosphate nanoparticles for drug delivery applications

Unlike other inorganic nanocarriers such as carbon nanotubes, quantum dots, magnetic nanoparticles, silica nanoparticles and metallic nanoparticles that increase mutation frequency, produce oxidative lesions, decrease cell viability and induce damage to DNA, calcium phosphates are the safest category of biomaterials. They offer several advantages over other nanoparticles such as having non-toxic degradation products, excellent biocompatibility,
*in vivo* and *in vitro* stability, and pH dependent solubility. Despite all of these advantages, synthesis of calcium phosphate nanoparticles in **porous** and non-agglomerated form has been an ongoing challenge in the field that has impeded the application of this category of materials in drug delivery and nanomedicine. The aim of this project is to synthesis calcium phosphate nanoparticles with high degree of porosity to be able to uptake substantial amounts of biomolecules.

(d) **Fabrication and in vitro characterisation of novel composition melt-derived bioactive glasses with antimicrobial properties.**

Bioactive glasses have been used in the clinical practice to fill and regenerate osseous defects due to their unique ability to bond to host bone and stimulate new bone growth. However, bioactive glasses have been lagging behind other bioceramics in terms of number of commercial products worldwide. It is quite challenging to design a glass composition that can be sintered without crystallisation but also remains bioactive. The aim of this project is to fabricate a new bioactive glass composition that has antimicrobial property and can be formed into 3D constructs without or minimal crystallisation.

(e) **Developing a facile technique to fabricate highly porous ceramics for bone tissue engineering.**

There is a current need for better bone graft substitutes to regenerate diseased or damaged bone. Ideally, the structure of the synthetic graft should be similar to that of trabecular bone, highly porous with interconnected pores. This is essential for cell attachment, proliferation, and migration for vascularisation and formation of new tissue. Moreover, porous structure facilitates nutrient and oxygen transfer that are key factors for health cell metabolism. There are variety of methods for producing porous materials such as polymer sponge method, robocasting or extrusion printing. The porous constructs made by such methods show either low mechanical strength or a pore structure that does not resemble the trabecular bone. The aim of project is to establish a facile method to produce strong porous scaffolds that mimics the trabecular structure of bone at complex anatomical shapes.

(f) **Bioactive ion delivery by calcium phosphate nanoparticles as a cue for stem cell differentiation.**

Incorporation of therapeutic ions into the structure of biomaterials for direct stimulation of cells is an attractive approach for tissue engineering strategies. The aim of this study is to fabricate calcium phosphate nanoparticles doped with specific ions to enhance chondrogenic differentiation of stem cells without using any growth factor and a possible treatment method for osteoarthritis.
My research group investigates how molecules interact with light, and the consequences, with applications ranging from studying radicals and ions of astrophysical and atmospheric interest, to renewable energy. Our principal tools are femtosecond and nanosecond lasers, with sophisticated detection schemes, vacuum chambers and mass spectrometers.

(a) Photochemical Upconversion for Improved Solar Energy Conversion

Light from the sun reaches us as a continuous spectrum. But, to generate a photovoltage in a solar cell, we usually neglect that part of the spectrum with photon energies below the band gap. Such a strategy limits the energy conversion efficiency of solar cells to about 33% (UNSW Si cells have reached 25%). Photochemical upconversion (PUC) can be harnessed to convert long wavelength into shorter wavelength light, increasing the photocurrent of the device.

Recently, we have applied PUC to amorphous silicon, organic polymer and dye-sensitized solar cells. But, efficiencies are still too low for application. To concentrate the absorption of light and increase upconversion efficiencies, we are currently exploring a range of nanostructured architectures incorporating biomimetic light harvesting materials.

(b) New Materials for Luminescence Solar Concentration (with A/Prof. Pall Thordarson)

One strategy to slash the cost of solar energy is to use a small area of solar cell and a large solar collector. However, usually such systems rely on geometric concentration of sunlight using mirrors. Such systems are expensive and cumbersome, and cannot concentrated diffuse light. The luminescence solar concentrator is promising way to do this using passive molecules.

When light falls on a slab of material containing fluorophores, light is absorbed but re-emitted isotropically. About 75% of this light is trapped in the slab by total internal reflection, and guided towards solar cells on the edge of the slab. Until now, such systems have been plagued by reabsorption effects. We will couple fluorescent dyes to light-absorbing nanomaterials to separate the roles of absorption and emission, and reduce reabsorption. Further improvements have been shown by us to be possible by clever design of the orientation of transition dipole moments.
Laser Spectroscopy of Isolated Radicals and Ions (with Prof. Scott Kable)
The new Molecular Photonics Laboratory houses sophisticated lasers and equipment with which we can discover new transient chemical species of importance in the gas phase chemistries of our atmosphere and the interstellar medium.

Atmospheric Radicals
One of the greatest scientific challenges of our time is to understand the complex chemistry of the atmosphere. Plants and human activity are responsible for >1000 Tg ($10^{12}$ kg) of volatile organic compounds being emitted into the atmosphere each year. These molecules are processed into less volatile compounds which then find their way into secondary organic aerosols, which are a major natural impactor on public health and climate. In this project, we will develop laser-based spectroscopic methods to detect and characterize intermediates formed on the way from the plant to the aerosol particle.

Interstellar Molecules and Ions
As stars die, they eject complex organic molecules into the interstellar medium, where they live out millennia before being incorporated into new stars and planetary systems. These organic molecules are the seeds of life, but, as yet, we do not know the chemical make up of the interstellar medium from which planetary systems are formed.

Using a star as a lamp, we can peer into this medium using telescopes by observing molecular absorption spectra. However, despite there being hundreds of nibbles taken out of the visible stellar spectra of stars occluded by diffuse clouds, only a few molecules have been unambiguously detected by their visible spectra. The unidentified features are known as the diffuse interstellar bands, and are the longest standing mystery in astrophysical spectroscopy.

In this project, we will develop techniques to capture the spectra of isolated, never-seen-before aromatic cations which the leading candidates for carrying the DIBs, and (hopefully) solve this long standing problem.

Advanced Spectroscopy for Complex Functional Materials (with Dr Dane McCamey, School of Physics)
Complex functional materials are employed in a range of applications, the development of which is motivated by the future technological needs of society. Organic solar cells, organic light emitting diodes and organic electronics all employ materials characterized by a complex relationship between morphology and function which can only be elucidated by advanced spectroscopic techniques.

Combining lasers and magnetic resonance, we will develop and apply new advanced spectroscopic techniques to complex functional materials, revealing the dynamical behaviour of charge carriers and excited states.
SOLID STATE AND MATERIALS CHEMISTRY

- We chemically tune the atomic arrangement (crystal structure) of solid state materials to enhance their physical properties such as energy storage capacity, ionic conductivity or thermal expansion.
- We use a combination of techniques to characterise our materials, including but not limited to X-ray and neutron diffraction (at the Australian Synchrotron and ANSTO), solid state NMR, electrochemical and impedance analysis, and electron microscopy.
- Our goal is to fully characterise materials, place them into real-world devices such as batteries and solid oxide fuel cells, and then characterise how they work in these devices.

It would be great to work with Honours students on the following projects:

(a) Towards the next generation of batteries: Sodium-ion batteries

Lithium-ion batteries are ubiquitous in our daily lives, e.g. mobile phones and laptop computers, but their limitations have restricted wide-scale use in applications requiring higher power, e.g. electric vehicles and energy storage of renewable energy. This project will target new battery chemistries, in particular sodium-ion batteries, by developing and characterising new electrode and electrolyte materials. We will work to develop a reliable and affordable room-temperature sodium-ion battery to provide sufficient power for large-scale energy storage from intermittent renewable power sources. Students will work on one of the following parts of a battery and test their component in idealized batteries.

Positive electrode materials

These electrodes provide the source of the sodium-ions and represent the largest cost and energy limitations for lithium-ion batteries. Here, new sodium-containing transition metal oxides, phosphates or sulfates will be synthesized and characterized to determine the relationship between crystal structure and battery performance. **We are working towards scaffolding layered electrode materials in order to dramatically improve performance.**

Electrolytes

Sodium-ion conducting ceramics or glassy-ceramics are known to be excellent electrolytes at high temperatures (>300°C). This project works towards making materials with sufficient sodium-ion conduction at room temperature.
**Negative electrode materials**

Negative electrodes are the least investigated component in a sodium-ion battery and the compounds used for lithium-ion batteries show poor performance in sodium-ion batteries. By developing new negative electrodes and understanding their limitations towards reversible sodium insertion/extraction we will be enable the next generation of devices.

**(b) Tuning negative thermal expansion to produce zero thermal expansion materials**

The majority of materials expand during heating via thermal expansion and this process is responsible for billions of dollars per year in maintenance, re-manufacture and replacement costs due to wear and tear on both moving parts (e.g. in aircraft gas turbines), and components that are designed to be static (e.g. in optics, coatings, electronics). If a zero thermal expansion (ZTE) material can be made, a material that neither expands nor contracts upon heating, this could dramatically reduce industrial costs. In order to achieve this, the opposite extreme of materials are considered in this project - negative thermal expansion (NTE) is a property exhibited by a small group of materials predominantly due to transverse vibrations of atom groups or cooperative rotations of units (e.g. –CN- or WO3). These materials typically feature large crystallographic voids and cations with variable oxidation states. So why not use a battery as a synthesis tool? In this project we will controllably insert Li and Na into the voids of the NTE materials, via a battery, in order to tune the cooperative rotations to produce ZTE materials.

**(c) Improving solid-state electrolytes by understanding their formation characteristics and phase evolution**

Safety is an important aspect of high power batteries. Using a solid-state electrolyte has significant advantages to the highly flammable liquid electrolytes that are commercially available. Unfortunately the ionic conductivities of solid-state compounds are generally lower than the liquid counterparts, especially under ambient conditions. At the other extreme, solid oxide fuels cells often operate at approximately 1000°C as the operating temperatures are essentially determined by the ionic conductivity of the electrolyte. In both examples, electrolyte ionic conductivity is a critical hurdle in preventing further development and use of these technologies. The ionic conductivity is directly related to the crystal structures adopted by the electrolytes and how they evolve with temperature. In this project lithium-ion and oxide-ion conducting materials will be synthesized and their ionic conductivities characterized. Importantly, variable temperature time-resolved neutron powder diffraction will be used to study the formation (from starting reagents) of these ionic conductors under varied conditions. This will shed light on the formation processes and optimal conditions required for synthesis.

**(d) Other projects**

Depending on your interests, other solid state projects, e.g. making new superconductors, can be designed. Please consult with Neeraj for further details.
My work is part of the Australian Center for NanoMedicine and ARC Centre of Excellence in Convergent Bio-Nano Science and Technology, led by Prof. J. Justin Gooding. The work that we have is revolving around the use of chemically modified polymeric material (both natural and synthetic) materials for biomedical and agricultural applications. It would be great to work with Honours students on the following project:

(a) Silk fibroin material for application in chronic wound healing for diabetic patients (in collaboration with Prof. George Mathew, Mochtar Riady Institute for Nanotechnology, Indonesia)

Recent work has showed that silk is a promising material for wound healing. It has shown to have a superior quality than commercially available product. The aim of this project is to further explore the use of silk as wound healing especially in diabetic patients with chronic wounds. As we all know, diabetes is one of the most prominent health problem especially in the developing countries and developed countries where the food nutrients contains high carbohydrate and high sugar dietary.

Wound bandages (such as gel or film, Figure 1) will be prepared from silk fibroin which has shown to promote skin cells growth. Moreover, we will also dope the bandages with antimicrobial compounds such as silver nanoparticles or diabetic drug. Once the proof of concept of the bandages has been performed, we will do the animal testing and further work in Mochtar Riady Institute for Nanotechnology and Siloam Hospitals located in Lippo Karawaci, Indonesia.

![Figure 1. Advanced materials from Bombyx Mori silk fibroin](image-url)
References

(b) Green and nature based material (chitosan) as preservatives for fresh food (in collaboration with Dr. Edgar Wong, UNSW, Universitas Gadjah Mada (UGM), and Salim Agro Group Company)

Food security is one of the grand challenges of our time. World population is projected to be 10 billion by 2050 which means food production needs to increase by 70% to be compared to the food demand in 2005. With the limitation of resources that the world have (land, finance, human, etc) we need to utilize the food that we produce the best we can.

The aim of this project is to investigate the use of chitosan as natural preservatives. You will we working with me and the team in UGM towards formulation that is safe, economical, scalable, and we will perform field trial in farms such as strawberries, chilies, or other fruits.
SCIENTIA PROF. MARTINA STENZEL
Level 2, Dalton Building (F12)
T: 9385 4656   E: m.stenzel@unsw.edu.au

NANOPARTICLES AND TAILORED POLYMERS FOR CANCER TREATMENT

- The delivery of drugs can be improved by packaging the drug into nanoparticles. Nanoparticles for drug delivery have typically sizes below 100 nm and can be prepared using various materials including polymers. In our group, we synthesize various polymers to create core-shell nanoparticles – the core holds the drug, mainly anti-cancer drugs, while the shell makes the particles soluble and determines the interaction with cells.
- In our group, we work on different aspects starting from organic synthesis to polymer nanoparticle preparation to testing these particles on cancer cell lines. We have meeting with clinicians and we discuss their drug delivery problems.

It would be great to work with Honours students on the following projects:

(a) Imitating viruses with polymers: Learning from the success of viruses

Most drug carriers described in literature are spherical nanoparticles. Interestingly, nature’s own highly successful nano-objects, viruses, have often elongated structures. Example is the by now well-known Ebola virus with its worm-like morphology. In addition, viruses carry bioactive groups that allow fast recognition of the host and quick entry. In this project, we will prepare elongated nanoparticles that will simulate the shape of viruses. To gain more understanding of the entry of these nanoparticles into cells, we will make nanoparticles of different softness as we have found that this could be a key parameter. The student will therefore spend some time with microscopy techniques such as AFM to evaluate the properties of the nanoparticle before studying cell uptake.

(b) Drug carriers inspired by nature: Nanoparticles with sugar antennae

Carbohydrates have become a hot topic for research within the scientific community. This is due to the myriad number of biological communication events, including: cellular recognition, inflammation, signal transmission and infection by pathogens displayed by them. To improve the distribution of drugs in a biological system, the use of a ligand (e.g. carbohydrate and peptide targeted therapeutics for the recognition of malignant cells), could be an important step towards the improved treatment of cancer and other diseases.
Synthesis of glycopolymers has been one of our core activities over the last few years. The polymers are prepared either by direct RAFT polymerization of glycomonomers or by post-functionalization of active polymers. These nanoparticles will be loaded with anti-cancer drugs and we like to learn how these nanoparticles interact with biological media such as proteins.

(c) Interaction of nanoparticles with cancer stem cells  
Collaboration with A/Prof Kris Kilian

Nanoparticles are quickly taken up by cancer cells. They can be used as vehicle to deliver drugs into cells in an efficient way. A lot is known about the influence of shape, size and other parameters on cellular uptake. This knowledge was gained by growing various immortal cancer cells in the lab. However, these cells do not resemble cell found in tumour where cancer cells may display enhanced tumorigenicity, mixed in with cancer stem cells. My colleague in the school of chemistry, A/Prof Kris Kilian has developed a model that allows us to grow cancer stem cells and cells of enhanced tumorigenicity on an engineered surface. Cells are grown on surfaces of different geometries such as coils and stars resulting in tumour tissue with a stem-cell-like phenotype. Incubation of these models with nanoparticles allows us to evaluate the rate of cellular uptake of nanoparticles by various phenotypes simultaneously. This can help us evaluating the differences in interaction of nanoparticles and help us identify what types of nanoparticles are suitable to target cancer stem cells or metastatic cells.

(d) Learning more about the structure of nanoparticles – Scattering analysis at ANSTO  
Collaboration with Dr Chris Garvey from ANSTO

When block copolymers self-assemble into micelles, it is widely assumed that the aggregate has a core-shell structure with a sharp transition between both phases. However, we do not know what the real structure is and how much water is in the nanoparticle. These properties however affect the biological activity. Small angle neutron scattering (SANS) and small angle X-ray scattering are excellent tools that provide more information. Once we understand the structure, we also understand why different nanoparticles behave differently and why some of them do not perform. In this project you would spend some time at ANSTO and learn and apply the technique. If time permits, you can even spend a day at the Australian Synchrotron in Melbourne. Prerequisite is some interest in mathematical modelling. Students are eligible to apply for a scholarship [http://ainse.edu.au/grad_students2/honours_scholarships](http://ainse.edu.au/grad_students2/honours_scholarships).
My group focuses on making and understanding new materials that are often focused on some of the major challenges facing us today: energy, water and sustainability. We make use of a range of techniques that include X-ray and neutron scattering in truly multi-disciplinary projects. Key to these studies is the notion of hierarchical emergent properties and complexity - the world around us derives from simple inter-molecular interactions; we aim for a greater understanding of these fundamental processes in order to deliver new materials displaying novel properties.

It would be great to work with Honours students on the following projects:

(a) **Metal organic frameworks (MOFs): coordination chemistry of the 21st century**

Over the last 20 years, inorganic chemistry has taken on board a number of new concepts and approaches that have reinvigorated the subject – one area showing particular promise is polymeric coordination compounds or MOFs. These topologically beautiful materials display intimate long range ordering and immense compositional flexibility, along with structural rigidity; they are ideal hosts for a range of molecular guests, opening up many potential applications.

**Sorting and storing molecules - how to select for one molecule over another**

This research project is specifically targeted at very real challenges faced in industry - effective separations of mixed gas streams and facile storage of gaseous fuels such as H₂. Highly porous MOFs make excellent host materials for small molecules such as CH₄ or H₂. By tuning their properties MOFs can become efficient storage vessels or effective gas-selective membranes such as the H₂ selecting MOF shown here.

**Quantum phenomena in magnetic materials**

Magnetic materials have revolutionised the way in which we store and use information and have a key role to play in quantum computing; they have also been a navigational aid for centuries and are even pretty useful at securing notes to the fridge door. It is fascinating therefore that we still do not fully understand the behaviour of such materials, especially when dimensionality is constrained. MOFs can have single chains (1D) or sheets (2D) of metal ions embedded into a non-magnetic matrix, making them ideal materials in which to study the effects of magnetic quantum confinement.
(b) **Order and disorder in molecular materials**

Solid state materials are often thought of in terms of the long range ordering of motifs into lattice structures; however what occurs upon phase transitions when molecular ordering may change or even order gives way to disorder? Welcome to the world of phase transitions, in which entropy and enthalpy play important roles in determining the behaviour of molecular motifs. Planar molecules, such as small aromatics, are of particular interest in that approximating to oblate discs, their reduced dimensionality directly influences their intermolecular interactions and orientations. They are also ideal systems to study; not too big, amenable to computational simulations, ubiquitous and very stable.

**Inter-molecular hydrogen-bonding**

Identified by Linus Pauling around 80 years ago, the hydrogen bond is the champion of intermolecular interactions, the basis of biology and our watery world. However there is a lot to still learn and to problems to study when it comes to H-bonding - we have been looking at a number of model H-bonded systems, making use of solid state NMR, X-ray and neutron diffraction and inelastic neutron scattering. This work is highly collaborative, requiring high-end research infrastructure and sophisticated numerical modelling - it is ideally to students with an inquisitive mind, seeking deep insights into the fundamentals of our every day life.

**Donor-Acceptor stacks: heterojunction photovoltaics to molecular magnets**

The intermolecular interactions between efficient electron donors (D) and acceptors (A) yield optically active charge transfer materials that can act as organic semiconductors, photovoltaics, ferroelectrics and light emitting diodes. Complete electron transfers can result in bulk magnetic materials. We aim to investigate the interactions of simple D...A stacks whilst modifying the peripheral functional groups, known to contribute to molecular packing. In this way, self-healing semi-conducting liquid crystalline materials can be produced that show remarkable anisotropy, enabling uniaxial conduction under greater load. With the wide range of suitable D and A molecules available, these materials have tremendous promise in their capacity to be tuned for specific applications, whether it be for emission in the visible spectrum (OLEDs) or broad-range absorption (OPVs). Being relatively small molecules, they are also suited to computational studies that are highly informative in terms of the electronic interactions and \( \pi - \pi \) stacking interactions.

(c) **Other projects**

Other projects involving materials-based chemistry, nanotechnology, graphene, crystallography and spectroscopy are available and can be tailored to your interests. Feel free to come and discuss possible research projects.
SYNTHETIC INORGANIC CHEMISTRY – LANTHANIDE COORDINATION COMPLEXES

Lanthanides are a commonly overlooked area of coordination chemistry – people often say “But we know everything there is to know and how they react”... This isn’t so, lanthanide complexes are incredibly interesting and have a range of potential applications. Lanthanides have uses in catalytic cycles, luminescent devices & interesting magnetic properties that could be utilised in data storage devices or qubits in quantum computing. This is where the research in the Sulway group comes in, we are exploring the synthesis and characterisation of new lanthanide containing coordination compounds that could be used in the technology of the future.

Skills you will learn:

- Manipulation of air- and moisture-sensitive compounds
- Organic and Inorganic synthetic chemistry
- Structure elucidation – NMR spectroscopy (\(^1\)H, \(^{13}\)C), IR spectroscopy, SQUID magnetometry and XRD (Yeap, we grow crystals)!

It would be great to work with Honours students on the following projects:

(a) Sterically hindered low-coordinate lanthanide compounds

Recent insight into stabilisation of the \(m_J\) states of lanthanide containing compounds hints at the potential ability to synthesis compounds that have higher energy barriers to magnetic relaxation than any 3d-block compound. It has been suggested that even subtle changes to the coordination environment can cause drastic changes in the magnetic behaviour of lanthanide containing compounds, simple things such as agostic hydrogen interactions to the metal centre can have profound results. Although most work has centred around synthesising high-coordinate compounds there have been several interesting observations of low-coordinate systems. This project involves synthesising and analysing a series of new low-coordinate lanthanide containing compounds that seek to exploit agostic hydrogen interactions to stabilise the \(m_J\) states of the lanthanide ions.\(^1\)
(b) Exploring novel linkages between lanthanide centres

As described in project (a) the smallest changes around a lanthanide centre can have dramatic changes to the magnetic behaviour of a compound. There have been a wide range of atoms used to bridge lanthanide centres but some of the more ‘exotic’ potential linkers are still unknown2... This is where you come in, this project is all about synthesising lanthanide containing compounds that have new linker molecules, we will be using a combination of ‘old school’ inorganic chemistry and organic chemistry to synthesis ligands that will allow us to go on and link lanthanides with such elements as P, Se and Te...

![Lanthanide complexes](image)

(c) Do you have an interest in education?

How about something a little different? Ask any academic about what aspect of their ongoing professional development often gets left by the wayside and it’s usually their teaching – this is not the case with me, I have a real passion for providing high quality teaching! And guess ‘what?’ you can research into chemical education too! My main research focus in education focuses on using the latest digital technologies to support and enhance learning, so if you feel passionate in this area then get in touch...

(d) Have your own ideas?

I’m open to discussing other potential ideas that you have after all it is your Honours year you should work on something you are interested in, just send me an e-mail...

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ORIGIN OF LIFE, COMPLEXITY AND NANOMEDICINE

- Origin of Life and Systems Chemistry, exploring the role of self-assembly in how life originated and how we can make life-like systems.
- Development of 3D Cell Culture materials for use in medical research and stem cell therapies
- Protein Chemistry and Self-assembly for better understanding of functional biological systems
- Complexity in Supramolecular Chemistry investigating the fundamental aspects of host-guest interactions
- Synthesis of novel peptides for nanomedicine, including drug delivery and tissue engineering

It would be great to work with Honours students on the following projects:

(a) Do liposome enhance the catalytic efficiency of RNA and peptides? (Collaboration with Scott Cohen – Children’s Medical Research Institute Westmead and Prof. Martin Van Kranendonk, BEES).

Recently, Origin of Life research has started to turn its attention to a new hypothesis for how complexity could have arisen from a the “pre-biotic soup” of chemical. Dubbed here the “geyser” model, it focuses on how hydration/dehydration (HD) cycles in a geothermal pond (fed by geyser activity), could generate liposomes that encapsulate peptides and/or RNA of increasing complexity with each HD cycle (See also the Front Cover article of the Scientific American in August 2017). One of the many questions that this model begs, is if the liposomal environment might enhance the catalytic activity of peptides and RNA. In this Honours project you investigate whether encapsulating catalytically active RNA or peptides in liposomes changes their catalytic activity. This project will not only give you insight into what is arguably one of the most important questions in science, i.e., how did life originate, but you will also gain valuable experience in synthesis, self-assembly and the chemistry of peptide and RNA biomolecules.

(b) Novel peptides for immunotherapy (Joint Honours Project with Dr. Angela Finch, SOMS, UNSW).
C5a is a potent inflammatory mediator generated by the activation of the complement system and has been implicated in the pathogenesis of as diverse range of inflammatory disorders. Cyclic C5a antagonists were developed based on the C-terminus of C5a. The most potent of these AcF[OPdChaWR] (PMX53) has nanomolar affinity for the C5a receptor (C5aR). PMX53 inhibits the activation of the C5aR in a non-competitive manner. The molecular basis of this non-competitive antagonism has not been established. To elucidate the mechanism of action of PMX53 fluorescent C5aR ligands need to be developed for use in kinetics binding assays. An understanding of the molecular basis of the actions of PMX53 will provide information for subsequent drug development.

(c) **Tropylium-based host-guest** (Joint Honours Project with Dr. Vinh Nguyen – School of Chemistry).

Tropylium is a $\pi$-electron poor 7-membered aromatic cation. Recent synthetic advances by the Nguyen group have made this unusual structural much more accessible, allowing us now to start to explore their potential in supramolecular host-guest. Their electron-deficient nature makes then particularly attractive for the binding and sensing of small and medium-sized biologically important anions such as chloride, phosphate and carbonates. We propose the synthesis of tropylium-based macrocycles (see figure) as the starting point for this project which will represent a new platform in supramolecular chemistry. Please also see Nguyen’s Honours projects for more details.

(d) **Nanomedicine: Smart soft peptide-based nanomaterials for medical applications** (collaboration with Dr. Adam Martin – School of Chemistry, Dr. Robert Norton in Biomedical Engineering and Prof. Maria Kavallaris, Children’s Cancer Institute Australia).

This work is aimed at designing and synthesising peptide-based smart soft nanomaterials for application in medicine, focusing on cancer-targeting peptides and peptide based materials for drug delivery, 3D-cell cultures, regenerative medicine and stem cell therapy. In collaboration with medical researchers across campus we are actively developing these systems as a potential tool studying neuronal cell with respect to Alzheimer’s disease, screening the activity of cancer drugs against cellular tumour model and controlling the growth of stem cells.

NANOPARTICLE SYNTHESIS & ELECTRON MICROSCOPY

Nanoparticles have unique properties controlled by their size and shape. In my research team, we focus on the solution chemical synthesis of nanoparticles with a focus of controlling nanoparticle shape and size.

It would be great to work with Honours students on the following projects:

(a) Iron nanoparticles for early detection of cancer

Early stage detection of tumours and cancerous cells requires the most sensitive and precise imaging of biological features in the body. Magnetic resonance imaging (MRI) and magnetic particle imaging (MPI) are the latest techniques that are non-invasive and provides 3D information with high levels of detail. In 2019 the University will be buying a new MPI system. The unique magnetic properties of iron and iron oxide nanoparticles make these ideal candidates for this state-of-the-art application. These key magnetic properties are linked to the size and crystallinity of the nanoparticles.

Using the leading edge of solution phase synthetic techniques, precise control over the nanoparticles and their magnetic properties can be achieved (Figure 2). In this project, well-defined nanoparticles with controlled crystalline domains will be studied for MPI. You will use transmission electron microscopy at one of the top microscopy facilities in Australia and be supervised by the director of the electron microscope unit, Professor Tilley. You will collaborate with leading researchers in MPI from Australia and internationally and work closely with a group of experts in nanoparticle synthesis. Overall, this work will tune nanoparticle size with precise synthetic control to optimise the magnetic properties of iron and iron oxide nanoparticles for MPI applications.
(b) Synthesis of shaped-controlled nanoparticles for renewable energy-storage

Developing a global-scale renewable energy that can fulfil the demand of billions of people without damaging the ecosystem is very crucial for securing our future energy. In general, water-splitting and fuel cell are the most promising technologies to convert the renewable energy source into chemical forms and then transfer it back to energy when it needs. Unfortunately, the large commercialisation of these technologies is still hindered by the high loading expensive noble metals. Therefore, the main goal is to develop active and stable catalyst in nano-scale to reduce noble metal loading.

Our strategy is to develop synthetic methods to control the size, shape and composition of nanocrystals, characterise them with advanced high-resolution transmission electron microscope (HRTEM) and then evaluate their electrocatalytic performance (such as ORR, OER and CO₂ reduction). We are exploring a wide variety metals such as Pt, Pd, Ru, Au, Ni and Co as well as its combinations and then systematically study the relation between catalytic performance and crystallography surface. We focus on fundamental understanding to design active and stable nanocatalysts to promote large commercialisation for water-splitting and fuel cell applications.

![Image of Ru catalysts synthesis and electrocatalytic performance](image)

*Figure of the synthesis, world record achieving Ru catalysts.*

(c) Probing “active sites” on nanocatalysts via high resolution electron microscopy

![HAADF images of nanocatalysts and EDX mapping](image)

*HAADF images of nanocatalysts and EDX mapping showing spatial information of their structures and compositions.*

With recent emerging challenges and opportunities in energy industry, nanocatalyst is one of the most investigated solutions for bringing an economically viable source of green energy. Due to the boom of nanocatalysts, the characterisation of these innovative materials has become more important than ever. Transmission electron microscopy is a powerful tool for us to understand the active sites on these nanocatalysts in atomic scale. With state-of-the-art electron microscopes provided by Electron Microscopy Unit, UNSW, we are able to obtain lots of structural and chemical information combining HR-TEM, STEM, HAADF, EELS, EDX, tomography and the advanced in-situ techniques. This valuable information will help us fundamentally understand how these catalysts work and empower us to rationally design next generation catalysts.
How did the first cell membranes on Earth self-assemble? How are swimming bacteria affected by obstacles? Surprisingly, some of the most fascinating and poorly understood phenomena in the natural world are at the mesoscale – too large to be understood as classical chemistry, yet still small enough to be subjected to the whims of thermal fluctuations and self-assembly processes.

Luckily, such phenomena can often be studied with a variety of cutting-edge microscopy methods. We use experimental techniques across science and engineering to collect data, and computational tools as much as possible for analysis. Many of the tools can also be adapted to study related questions in other fields of science.

I am starting as a Scientia fellow and anticipate having access to lab resources to undertake the following projects as early as Term 2 in 2019. There is potential for collaborations with labs in the United States and Asia. I’m available to chat about timing and potential projects (including but not limited to those listed below) via Skype. I am interested in helping students learn research skills, but also tailor their experience to their career goals and interests.

**It would be great to work with Honours students on the following projects:**

**(a) Extracting *E.coli* swimming behaviour from holograms**

Wild-type *E.coli* swim at tens of body-lengths per second, and rotate (‘wobble’) at over 20 Hz. Their swimming strategy is known as the canonical ‘run and tumble’, and is a key model system for understanding microorganism motility.

We recently demonstrated that ‘run and tumble’ can be captured using a fast, three-dimensional imaging technique – digital holographic microscopy – offering unprecedented tracking precision and time resolution [1]. These are digital version of the shiny stickers you might be familiar with. However, the analysis involves inverse-modelling using light-scattering solutions, and is computationally quite expensive.

This project will involve developing new analysis tools to extract information about how *E.coli* swim from digital holograms. Developments could lead to a longer project aimed at understanding how bacteria move through obstacles consisting of different stimuli, and an improved understanding of microorganism motility. It can also extend to studies of other organisms. A background in Python will be useful but not necessary.

**(b) A ‘warm little pond’ dries out – crowding of model protocell membranes**

Wet-dry cycles are postulated to be an important part of the physico-chemical processes that gave rise to life on early Earth. The role of wet-dry cycles in creating complex macromolecules is being
extensively explored in other research groups, but what happens to the compartments in which the molecules are housed?

This project will investigate what happens when a population of model primitive cell membranes are subjected to drying. In addition to the protocells being crowded, what else might happen? The dynamics will be captured with microscopy, and the role of the air-water interface will be characterised with a custom-built pendant-drop tensiometer.

This project has applications in understanding the origins of life. There are also implications in soft matter science, where the crowding and jamming of hard colloidal particles have been studied extensively but the behaviour of ‘soft’ particles such as vesicles are not as well-understood. The pendant drop apparatus can also be adapted to investigate other phenomena in interfacial sciences, such as creating microfoams for your favourite milky espresso drinks.

(c) Coupling membrane growth with permeability in model protocell membranes

Modern cell membranes are mostly comprised of phospholipids, and regulate what enters and exits the cell with complex protein machinery. Without specialised protein channels and transporters, phospholipid membranes are impervious to most small molecules. Logic thus dictates that prior to the evolution of such machinery, primitive membranes must have been more permeable than their modern counterparts to access nutrients from the environment.

This project aims to understand how primitive membranes could have tuned their permeability with their composition. We will screen how potential candidate molecules for primitive cell membranes, including fatty acids, fatty alcohols, alkanes, and polyaromatic hydrocarbons, affect membrane permeability to uncharged molecules such as sugars, and small charged molecules such as mononucleotides.

Select membranes will then be subjected to competitive growth with each other. These experiments will determine how membrane composition couples permeability with growth, providing potential selective advantages on early Earth.

CLEAN ENERGY TECHNOLOGIES AND ELECTROCHEMICAL SYNTHESIS

Clean, renewable energy has enormous implications for the future prosperity of humankind. As a thriving civilisation, living better and longer has been our instinctive pursuit, and advanced biomedical technology is therefore always highly demanded. Research in our lab addresses these problems by using electrochemical technology, nanotechnology and biotechnology. Our research areas include solar water splitting, CO₂ reduction, gas sensors, cochlear implants, bioimaging, and flexible batteries.

It would be great to work with Honours students on the following projects:

(a). Solar Hydrogen Fuel Production From Seawater

Production of hydrogen fuels from water using electricity generated from renewable energy sources such as solar and wind can provide a sustainable and clean fuel supply for human use. Conventional water splitting is typically carried out in freshwater containing an added supporting electrolyte to conduct electricity, such as potassium hydroxide. However, freshwater only represents a microcosm of the total forms of water found on Earth. The vast majority of water on Earth is seawater (approximately 97%), which contains naturally present salts, predominately sodium chloride. Current hurdles in seawater electrolysis lies in the release of toxic chlorine gas due to the kinetically favoured chlorine evolution over oxygen evolution. The project will develop novel electrodes made of Earth-abundant materials and a prototype water splitting cell for hydrogen production directly from seawater without chlorine evolution.

(b). Conversion of CO₂ to Fuels with Renewable Electricity and Earth Abundant Catalysts

Fossil fuels have historically been the primary feedstock for petroleum based products and industrial chemicals. Apart from the impact that fossil fuels pose on the environment, they are generally mined in remote locations and require massive infrastructure for processing and distribution before they are even refined. One promising solution is to reduce CO₂ itself to petrochemical feedstock, which could cater to the unprecedented consumerism of society and simultaneously reduce the anthropogenic emissions of CO₂ in the atmosphere to restore the natural carbon cycle. To improve the CO₂ reduction efficiency, advanced catalysts that are efficient, selective, stable, and low cost need to be developed. This project will design a class of inexpensive, non-metallic electrocatalysts based on nanoporous graphene. The electrocatalysts will be integrated into a prototype device for converting CO₂ into useful fuels.
(c) Electro catalytic Synthesis of Ammonia from Renewable Hydrogen and Atmospheric Nitrogen

Ammonia is an important commodity in future hydrogen economy due to high energy capacity and ease of storage and transportation. The Haber-Bosh process is vital for the fertilizer industry due to a high rate of ammonia production but non-ambient conditions, energy intensive nature and sophisticated infrastructure requirement hampered its utilization as green and decentralized system. Electrochemical nitrogen reduction reaction (NRR) at ambient conditions powered by renewable energy sources is the alternative towards sustainable chemistry.

This approach is currently limited by competitive hydrogen evolution reaction (HER) and low rate of ammonia production. Effective control of material's architecture at nanoscale could lead to the development of improved materials with tailor-made physical, electronic and chemical properties. Our group has recently made breakthrough in developing metal-organic framework (MOF) based catalyts for NRR. In this project, the student will have opportunity to work on these advanced electrocatalysts and evaluated their performance for ammonia synthesis using renewable electricity, hydrogen and atmospheric nitrogen.

(d) Nonprecious Metal Catalysts for Hydrogen Fuel Cells: Towards Affordable Hydrogen Powered Electric Vehicles

Hydrogen fuel cell powered vehicles have haven regarded to be the ultimate solution to the future of transportation, with pure battery electric vehicles better suited to smaller cars and suburban needs. Low-temperature hydrogen fuels cells producing electricity using hydrogen and air, with water as the only by-product offer the advantages of simplicity and zero greenhouse gas emission. However, an affordable low-cost fuel cell with catalysts capable of working at industrial scales is yet to be developed. The primary challenges for this project are to discover low-cost electrocatalysts that are active and stable to replace the benchmark catalysts based on precious metals such as platinum for cathode catalyst for hydrogen fuel cells.

In this project the student would learn how to synthesise mesoporous nonprecious metal catalysts. The student will learn how to assemble, prepare and test a hydrogen fuel cell. The student will also have the opportunity to characterise the nonprecious metal catalyst materials using a range of characterisation techniques (XRD, TEM, XPS), and their electrochemical behaviours in operating hydrogen fuel cells.
HONOURS
ALTERNATIVES
Honours Practicum at King's College London

As part of the PLuS Alliance, we are now able to offer the possibility of completing an Honours projects at King's College London (http://www.kcl.ac.uk/nms/depts/chemistry/index.aspx).

With a pedigree as one of the oldest Chemistry Departments in England, King's Chemistry enshrines the rigour of the discipline in a progressive context. Continuing an illustrious tradition at the University, epitomised by the discoveries of Rosalind Franklin and Maurice Wilkins in the structure of DNA, the department has a distinct focus on understanding the chemistry of life and the interface with Biology.

King’s provides a vibrant environment in which to study 21st century Chemistry in the heart of London.

Students will be enrolled in Honours at UNSW, but will complete their projects in London under local supervision. Grades will be transferred to UNSW and students will graduate with Honours from UNSW.

The practicum program provides the opportunity for those keen to extend themselves in both their research project and life beyond the lab.

Students interested in this opportunity should speak to A/Prof. John Stride after exploring the King's College website and identifying potential supervisor(s).
Research into chemistry is also conducted within the School of Physical, Environmental and Mathematical Sciences at the Canberra campus of UNSW. Co-located with the Australian Defence Force Academy, UNSW Canberra maintains a diverse research program and is home to many research students. It is straight-forward for current UNSW Bachelor of Science students to transition to the Honours program at UNSW Canberra.

A selection of the chemistry research areas being actively pursued at UNSW Canberra are listed below, organised by research group leader. A range of Honours projects are available within each group, which can be adjusted to fit a student's interest. Group leaders may also be available for collaborative projects with research groups within the School of Chemistry, on a case-by-case basis.

Students with an undergraduate Weighted Average Mark (WAM) of 85 or higher are eligible for an $8000 Honours scholarship if enrolled at UNSW Canberra.

Students who complete their Honours degree within the School of Chemistry should also consider the possibility of higher degree research at UNSW Canberra, as the research at this campus extends into areas complementary to those actively pursued within the School of Chemistry. PhD scholarships for study at UNSW Canberra are generally available to all UNSW students who achieve First Class Honours.

**Bio-inorganic Chemistry — Prof Grant Collins**

The current focus of our work is in the development of new, and very promising, classes of multinuclear ruthenium complexes as antimicrobial agents. The emergence of drug-resistant populations of microorganisms means there is clearly a need for the development of new antimicrobials — but more importantly, there is the need for the development of new classes of antimicrobials. Complementing the antimicrobial studies has been research on the toxicity and the biological processing of the ruthenium complexes in eukaryotic cells. Emerging directions include utilising ruthenium complexes more broadly as anti-parasite agents, particularly in the treatment of schistosomiasis.

**Supramolecular Chemistry — Dr Anthony Day**

The research interests of the Supramolecular Chemistry group are based in organic chemistry synthetic design and the development of new synthetic techniques – in particular molecular host/guest chemistry. The family of molecular hosts known as cucurbit[n]uril and derivatives of this family are a particular target. Specific areas of research interest involve drug delivery vehicles, sensors and supramolecular materials.

The group has a secondary research area involving energetic materials, including insensitive munitions, detection, deactivation and environmental aspects. Applied aspects of this work with the Australian Defence Force and the Australian Federal Police are supported by strong links within the research team.
Theoretical Chemistry — Dr Terry Frankcombe

The group’s research activities fall broadly under the umbrella of theoretical and computational chemistry, extending into chemical physics. Four main research themes are currently being pursued: Gaussian-based quantum dynamics methods, gas–surface dynamics, dielectric materials, and the structure and mechanism of photosystem II. Secondary areas of investigation are processes occurring on the surfaces of spacecraft, simulating condensed matter spectroscopies, and “divide-and-conquer” strategies. Our research can be computationally intensive and involves the combination of chemistry, physics, mathematics and computer science.

Beyond these focus areas the group maintains active expertise in quantum chemistry in general, in molecular, condensed phase and surface adsorbate contexts.

Optical and Laser Spectroscopy of the Solid State — Prof Hans Riesen

The research of the Riesen group has been mostly focused on laser spectroscopy of transition metal ion doped insulators/wide band gap semiconductors. We are particularly interested in light-induced changes in the solid state that have potential applications in ultra-high density optical data storage and optical signal processing. Very recently Hans and some of his team have studied the generation of slow and fast light by transient hole-burning.

With the advent of the Australian Synchrotron, Hans has also become a user and strong supporter of synchrotron science. In recent years, the group have discovered a novel X-ray storage technology with applications in personal and clinical dosimetry, and medical imaging.

Inorganic Chemistry and Electrochemistry — Dr Lynne Wallace

The Wallace group research interests include the synthesis and study of redox-active and luminescent transition metal complexes, and applications of such complexes in sensor systems, light-activated molecular devices, supramolecular assemblies and therapeutic approaches. Electrosynthesis of green energetic materials is also a research focus.

Statistical Mechanics — Assoc Prof Cliff Woodward

The Woodward group conducts research in the field of statistical mechanical theories of condensed matter and complex fluids.

Some highlights of our research program include density functional theory and simulations of room temperature ionic liquids and polymer mediated interactions in polymer/particle mixtures, including many-body effects close to criticality. We have also used intensive simulations and theory to investigate biological systems, in particular, the riddle of “arginine magic”; the poorly understood mechanism that allows arginine-rich peptides to easily penetrate cell membranes. While most of the theoretical work carried out in the group is not reliant on massively large computational platforms, potential candidates should have a strong background in computational methods, physics or physical chemistry and mathematics.
JOINT PROJECTS AND COLLABORATIVE PROJECTS WITH OTHER SCHOOLS ACROSS UNSW

School of Chemistry researchers collaborate broadly with researchers in other Schools, Faculties and Institutes. If you are a Chemistry major or are eligible for Honours and wish to do a project aligned between Chemistry and another discipline, please contact the Honours coordinator.