Bachelor of Science (BSc)

BSc Advanced Science

BSc Medicinal Chemistry

Honours in Chemistry 2021

Never Stand Still | Science | School of Chemistry

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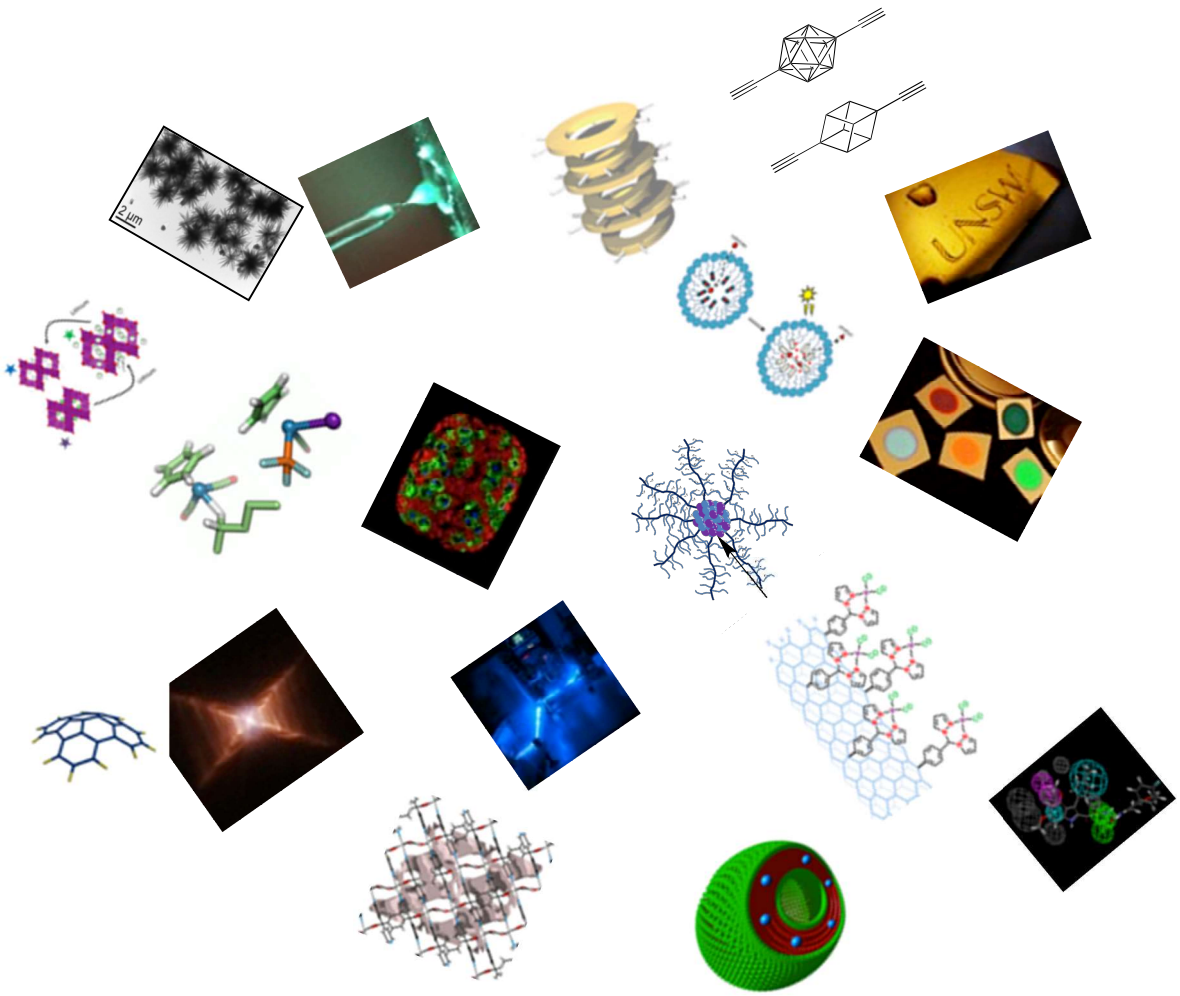
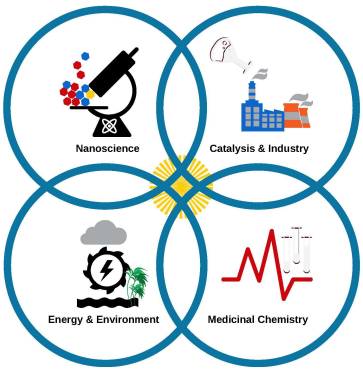


WELCOME

The School of Chemistry at UNSW is one of the leading centres of chemistry research in Australia. Composed of around 30 well-funded **research teams**, we are located in the following buildings on lower campus: Dalton (F12), Chemical Sciences Building (F10NA and F10), Hilmer Building (E10) and the Science and Engineering Building (SEB). 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 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)

Associate Professor 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.

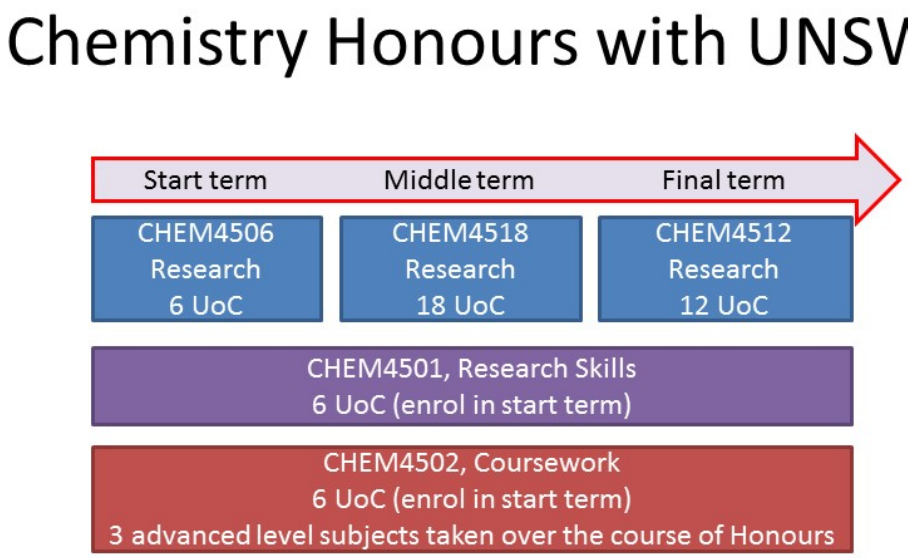
HONOURS IN THE SCHOOL OF CHEMISTRY

In 2021 the School of Chemistry offers Honours programs that are suitable for students enrolled in **Science, Advanced Science, Medicinal Chemistry and Environmental Science or *with a related undergraduate Science degree*.** 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.

We welcome all Science graduates from all over the world to apply to our Honours programs. You can start in any term of the year.

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.



Students log on to 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 are a combination of either theory, skills or both.

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 for the Thursday 12 pm seminars 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), consult the School of Chemistry Research Booklet (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). 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, Associate Professor 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. Details are available from the Honours Coordinator (Dr Neeraj Sharma).

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 (%)

Class 1	85+
Class 2 Division 1	75 – 84
Class 2 Division 2	65 – 74
Class 3	50 – 64


2000

HONOURS SUPERVISORS

A/PROF. GRAHAM BALL

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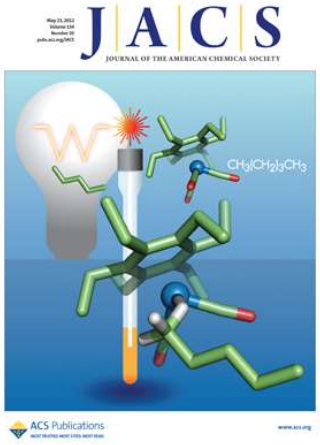
NMR SPECTROSCOPY AND COMPUTATIONAL CHEMISTRY: APPLICATIONS TO ORGANOMETALLIC AND BIOLOGICAL CHEMISTRY

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 biolmolecular 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

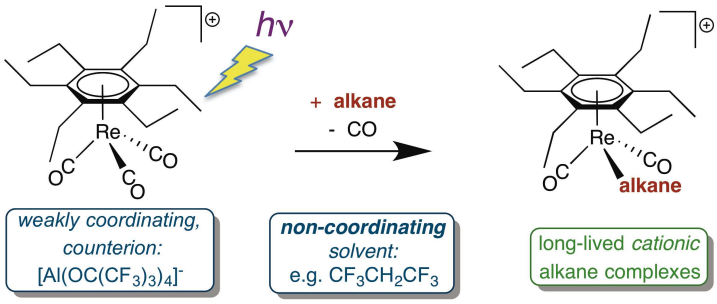


What should we do with petrol? Mostly it is just burned as fuel leading to damaging CO_2 and a rapid dwindling of this precious resource that took millions of years to form. Recently, chemists around the globe have been working on ways of converting relatively unreactive alkanes found in petroleum into 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 complex[1,2,3] including the *JACS* cover above[1] 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.

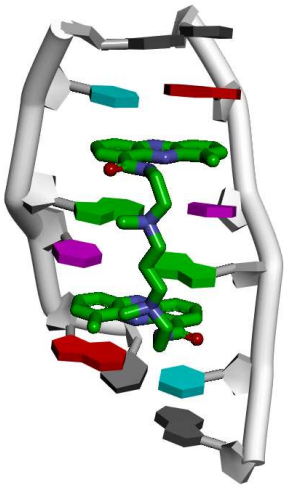
1 Young, R.D.; Lawes, D.J.; Hill, A.F.; Ball, G.E. *J. Am. Chem. Soc.*, **2012**, *134*, 8294. Podcast at http://pubs.acs.org/JACSbeta/coverartpodcasts/ #38.

2 Yau, H.M; McKay, A.I; Hesse, H.; Xu, R.; He, M.; Holt, C.E.; Ball, G.E. *J. Am. Chem. Soc.* **2016**, *138*, 281.

3 Young, R.D.; Hill, A.F.; Hillier, W.; Ball, G.E. *J. Am. Chem. Soc.*, **2011**, *133*, 13806.

4 Ball, G.E.; Darwish, T.A; Geftakis, S.; George, M.W.; Lawes, D.J.; Portius, P.; Rourke, J.P. *Proc. Natl. Acad. Sci. USA.*, **2005**, *102*, 1853.

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



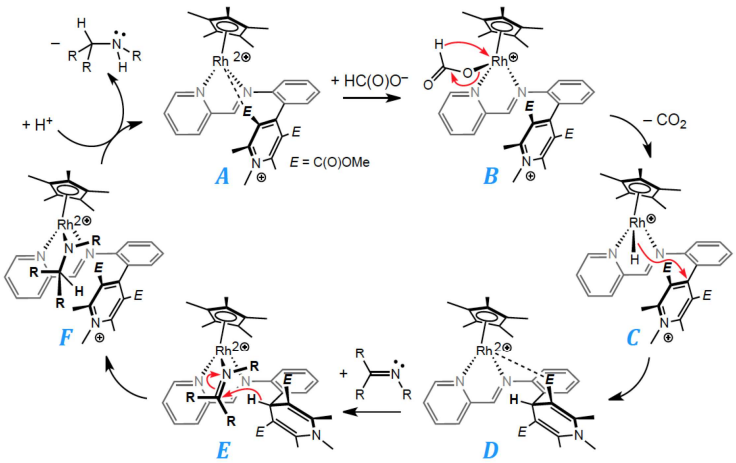
DNA presents one of the most logical and practical targets for anti cancer therapeutics. We are investigating the binding of several bis-intercalating molecules that show promise as next generation anti-cancer drugs and also the binding of clinically established drugs such as mitoxantone. The solution 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.

5. Serobian, A.; Thomas, D. S.; Ball, G. E.; Denny, W. A.; Wakelin, L. P. G. *Biopolymers* **2014**, *101*, 1099.

(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 CO_2. 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.



6. McSkimming, A.; Chan, B.; Bhadbhade, M. M.; Ball, G. E.; Colbran, S. B. *Chem. - Eur. J.* **2015**, *21*, 2821.

DR. JON BEVES

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SUPRAMOLECULAR AND COORDINATION CHEMISTRY

Our research involves using the weak interaction *between* molecules to control their function, with a particular focus on using *visible light* to change the properties of colourful molecules. All projects involve some synthesis, and usually NMR spectroscopy to study structure and properties.

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

(a) Photo-driven molecular machines

(collaboration with Prof. Ben L. Feringa and Dr Sander Wezenberg, University of Groningen, Prof. Dean Astumian, University of Maine)

We are designing and synthesizing small molecules capable of performing tasks such as controlled motion or selective binding. At particular goal is to control the diffusion of molecules so we can *direct their movement using light* (e.g. with an LED torch), which would offer the potential for applications ranging from pollution remediation to control over biological function.

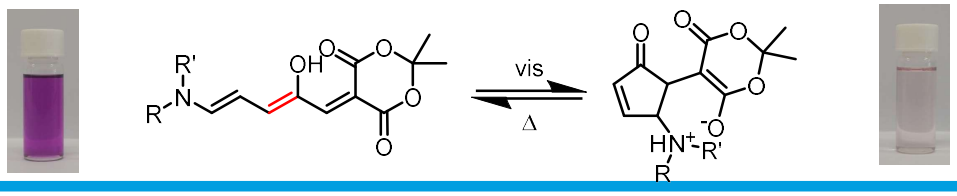
Skills: *organic synthesis, NMR spectroscopy, absorption/emission spectroscopy, kinetics…*

Relevant publications: *ChemPhysChem*, **2019**, DOI: 10.1002/cphc.201900150

(b) Molecular photoswitches

(collaboration with Prof. Joakim Andreasson, Chalmers Institute of Technology, Sweden and Prof. Nathan McClenaghan, University of Bordeaux, France)

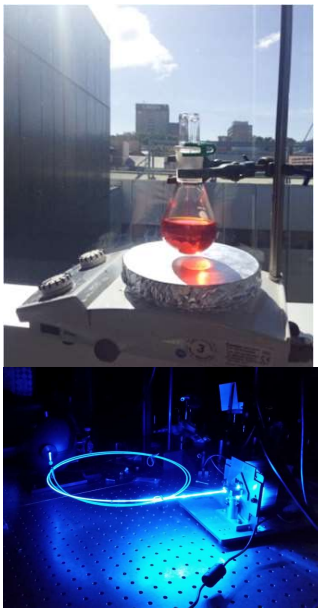
Some types of organic molecules can be isomerised between two forms using light. These two forms typically have very different properties, such as polarity, pK_a and reactivity. We are looking to use visible light switchable molecules to control molecular reactions, such as driving pH changes or switching ON/OFF catalytic activities. Two classes are currently being studied in our group: donor-acceptor Stenhouse adducts (DASAs) and various azo-compounds, such as heteroarylazobenzenes. We



synthesize these compounds typically in a few steps and investigate their fascinating switching behaviour and how this can be used to control properties such as pH, reactivity or guest release.

Skills: *organic synthesis, multidimensional NMR spectroscopy (including photo-NMR), absorption/emission spectroscopy, kinetics,…*

Relevant publications: *Chem. Sci.* **2018**, 9, 8242-8252; *Chem. Commun.*, **2016**, *52*, 13576-13579



(c) Photoredox catalysis

(in collaboration with Dr Evan Moore, UQ)

The use of visible light to catalyse reactions, generally using transition metal complexes, has developed into a major area of research in the past decade. Despite the practical use of common photoredox catalysts in organic synthesis, their performance and the mechanisms of the reactions they catalyse remain very poorly understood. This project will take a "coordination chemistry" approach to the problem, characterising essential redox and photophysical properties of viable photoredox catalysts and correlating these values with synthetic performance.

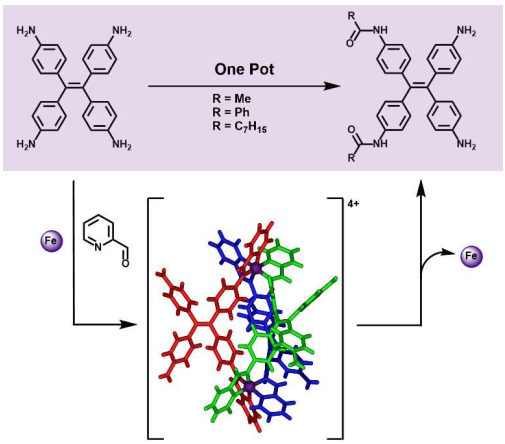
Skills: *organic and inorganic synthesis, NMR (including photo-NMR), cyclic voltammetry, X-ray crystallography, photophysical measurements,…*

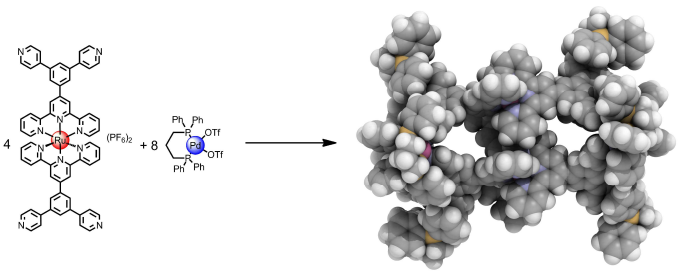
Relevant publications: *Polyhedron*, **2019**, 1-9; *Inorg. Chem.*, ***2018***, *57, 8476–8486*; *Inorg. Chim. Acta*, **2017**, *458*, 122-128; *Inorg. Chem.*, ***2016***, *55, 12737−12751*; *Chem. Commun.*, ***2015***, *51, 4465 – 4468*.

(d) Self-assembly of functional structures

(in collaboration with Dr Anthony Day, UNSW Canberra)

Using appropriately designed molecular components, large and symmetrical structures can be formed by "self-assembly" upon simple mixing of the different components. The resulting structures can exhibit remarkable properties, especially when constructed using transition metal complexes. This project will build useful redox- and photo-properties into these ordered structures, either as components (as in the two examples shown) or by the encapsulating metal complexes within organic hosts to tune their properties.





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

Relevant publications: *Chem.- Eur. J.* **2019**, DOI: 10.1002/chem.201806259; *Org. Lett.*, **2017**, *19*, 4034-4037; *Chem. Commun.*, **2015**, *51*, 4465 – 4468.

(e) …other projects tailored to your interests!

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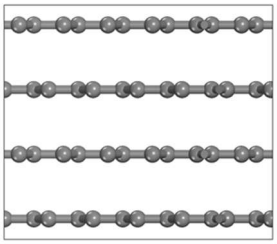
ADVANCED MATERIALS AND NANOTECHNOLOGY

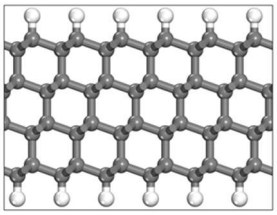
Chen's research focuses on advanced materials, particularly through the development of new synthesis strategies and applications of multidimensional carbon materials. The core of Chen's research is the development of new materials and understanding of properties of materials, especially carbon-based nanostructures including graphene, graphene oxide, reduced graphene oxide, amorphous carbon, diamond, “curved” carbon, fullerenes, nanotubes, nano-onions, “peapods”, carbon foams, films and membranes, as well as relevant 2D materials and nanostructures.

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

(a) Discovering new forms of nano-carbons



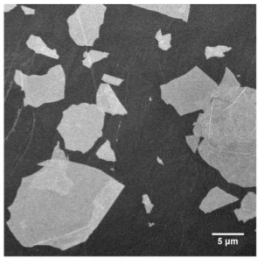
a



b

Carbon is arguably the most important element that provides the basis for life on Earth. Thirty-four years on from the ground-breaking discovery of buckminsterfullerene (C_{60}), the remarkable potential of low-dimensional carbons, including fullerenes, carbon nanotubes and graphene, have brought an entirely new era of carbon allotropes and defined their overwhelming scientific and technological significance. Looking into the future, several types of nano-carbon allotropes that have been theoretically predicted have not yet been experimentally achieved. This Honours project targets a challenge of synthesising diamond-like thin films through ion implantation of carbon into metal substrates. The experimental realisation of such materials, as well as an increased understanding of their structures and properties is highly compelling at both a fundamental and technological levels.

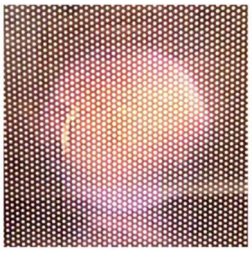
(b) Water permeation through membranes of 2D materials

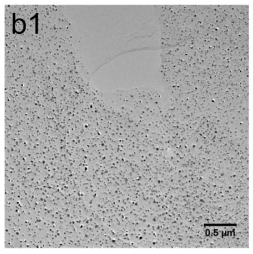


Ultrafiltration and nanofiltration are membrane-based filtration processes that rely on the design of the new membrane materials and technologies that are low cost and energy efficient for water treatment. In recent years, significant advances in the understanding of mass-transportation in nanochannels and nanopores have allowed for a new class of two-dimensional (2D) membranes whose performance surpasses conventional membranes. 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. The application of new membrane-based technologies includes filtration of waste/contaminated water and seawater desalination.

(c) Graphene-based materials for energy applications





Graphene is essentially a single layer of graphite. What makes graphene special is its sp^2 bonded nature and atomic thinness. These properties offer graphene to possess many material records in terms of thinness, strength, electricity and heat conductivity, and many others. Indeed, graphene is a "miracle" material in the current research fields of materials science, chemistry and physics. This Honours project involves the development of a new microwave induced shock processing strategies of graphene and the preparation of graphene with various structures such as nanoparticle decorated graphene and heteroatom doped graphene. A domestic microwave oven that is used for cooking/heating food in kitchen everyday can be used to prepare a large quantity of this "superstar" (very expensive) graphene material. The prepared graphene-based materials will be applied in energy-related applications, including batteries, electrocatalytic water splitting, fuel cells and CO_2/ N_2 reductions.

(d) Nano-carbons for biomedicine

Water soluble nano-carbon materials, such as graphene oxide and carbon quantum dots, exhibit excellent colloidal properties and potential for surface functionalization, attractive for use in biomedicine, including tissue engineering, antimicrobial agents, bioimaging, and drug delivery. In this Honours project, different multidimensional forms of nano-carbon and the different carbon-based materials made by chemical modifications or by combination with relevant bioactive molecules and nanoparticles will be developed and used for therapy, imaging, diagnosis and theranostics.

These projects are based on experiments in chemistry laboratory, which will require the use of advanced microscopic and spectroscopic techniques at the UNSW Mark Wainwright Analytical Centre (http://www.analytical.unsw.edu.au/) for material characterisation. These include transmission electron microscopy, scanning electron microscopy, atomic force microscopy, X-ray diffraction, Raman spectroscopy, X-ray photoelectron spectroscopy, etc. Depending on the research project, the candidate will be supported for training and accessing these instruments.

I am also open to discussions on other project ideas that you are interested in the "nano playground". Feel free to send me an email or just simply drop by my office in Dalton 125.

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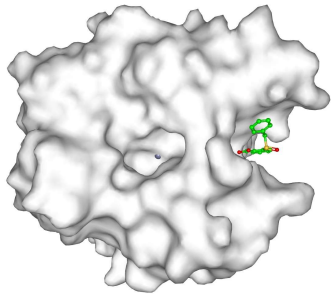
FUNDAMENTAL & APPLIED MASS SPECTROMETRY

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) 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.



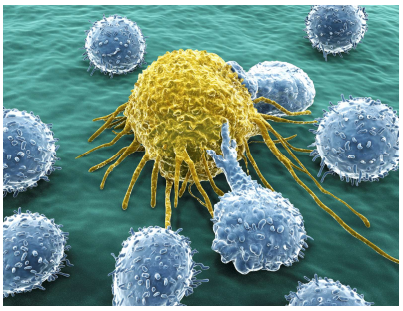
Where does the drug bind? Methods for rapidly pinpointing where small molecules bind to druggable targets are urgently needed for discovering the next generation classes of bioactive molecules.

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.

(b) Single-cell chemical analysis by mass spectrometry

We are interested in answering the fundamental question of what makes a cancer cell a cancer cell? Why are some cells drug-resistant while others are susceptible? Why do some metastasize while others do not? Not every cell was created equal. Individual cells within a population can be as dissimilar as the members of human families. Thus, we need to be able to perform chemical analysis on the contents of single cells, which requires the development of powerful analytical methods that have unprecedented sensitivity and selectivity.

For single-cell chemical analysis, mass spectrometry is one of the most promising analytical techniques because it enables many different types of molecules to be rapidly detected and identified nearly



Single-cell mass spectrometry: What makes a cancer cell a cancer cell? Powerful analytical methods must be developed to enable the contents of single cells to be identified and quantified with unprecedented sensitivity and selectivity.

simultaneously from exceedingly small sample volumes. However, matrix ion suppression is a key challenge that hinders the ability of scientists to detect the vast majority of metabolites and biomolecules in human cells. Recently, we have developed a novel, surface-selective ionization approach that enables trace chemicals to be rapidly detected from complex mixtures with minimal ion suppression using mass spectrometry.

In this project, you will take this research to the next level by fabricating novel surface-enhanced microprobes to sample and analyse the contents of single cells by a range of mass spectrometry techniques to target important disease biomarkers. The success of this project will provide a rapid, high-throughput platform to characterise a wide variety of important biomarkers expressed uniquely in each cell, with the goal of understanding how cellular heterogeneity leads to disease states and drug resistance.

(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 complex mixtures.

Portable mass spectrometer for personal chemical analysis: The ultimate device for preventative medicine? New and improved field deployable ionisation methods are urgently required to enable complex mixtures to be directly analysed (*e.g.*, for early detection of cancer and other diseases). *J. Am. Soc. Mass Spectrom.* **2008**, *19*, 1442-48.

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.

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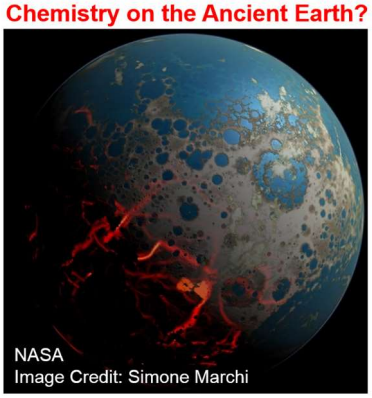
ORIGINS OF LIFE CHEMISTRY RESERACH

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 simple conditions (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.

Chemistry on the Ancient Earth?

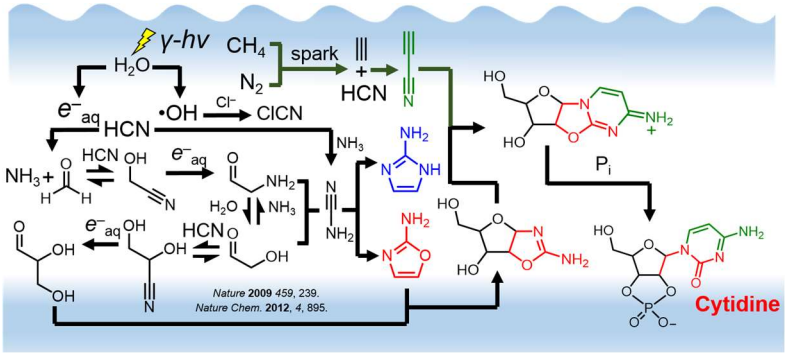


I am a new Lecturer starting in the School of Chemistry ready to take on students. Students may have potential opportunities to collaborate with and visit scientists from NASA Astrobiology labs in the US, as well as researchers from the Earth-Life Science Institute at the Tokyo Institute of Technology 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

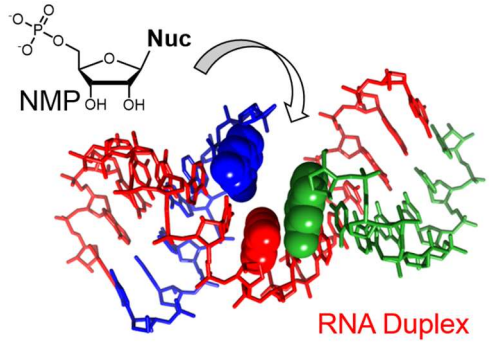
The need to make, measure and model complex reaction networks, especially those that give rise to hypothetically relevant prebiological compounds like ribonucleotides and amino acids, is fundamentally important for addressing the chemical mysteries shrouding life's origins. The goal of this project is 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, cyanamide, 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

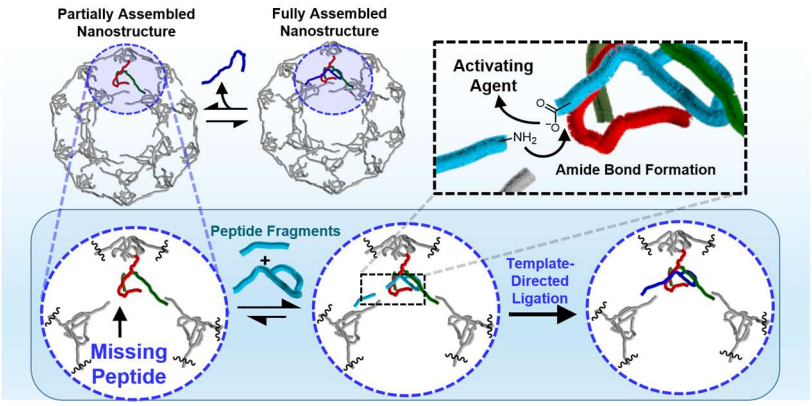


RNA is often hypothesized to be among the first genetic polymers to have arisen abiotically from chemical evolution on the early Earth. The template-directed replication of RNA – without the aid of modern enzymes – offers a mechanism by which Darwinian evolution may have originally initiated. The objective 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!

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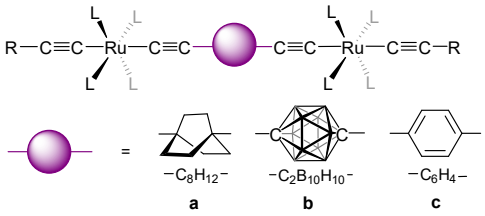
SYNTHETIC ORGANOMETALLIC CHEMISTRY

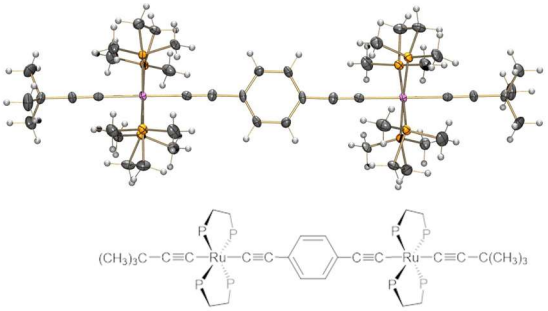
- Research in the Field group is centred around synthetic organometallic chemistry:
  - Development of organometallic catalysts that are able to activate small molecules (such as N_2, CO_2, *etc*), and to functionalise organic hydrocarbons (CH_4, ethylene, acetylene *etc*) to make value-added products, and perform specific organic transformations.
  - Development of organometallic polymers for application in areas such as molecular conductors, molecular semiconductors and 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 (^{31}P, ^{15}N, ^{29}Si, ^{19}F), 2D NMR spectroscopy, IR spectroscopy and X-Ray diffraction.

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

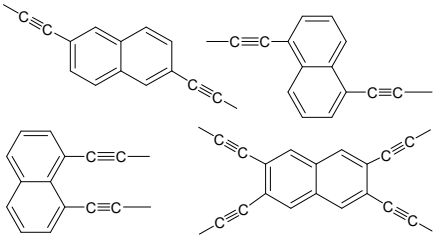
(a) Organometallic Polymers

Organometallic compounds containing complexed metals linked by bridging groups have many potential applications in materials science. We are particularly interested in the use of unsaturated organic groups (*e.g.* alkynes and arenes) as the bridging units and we are developing new methods for forming metal complexes where the metal centres are bridged by organic acetylides. Acetylide-bridged organometallic complexes show interesting electrochemical behaviour, and electronic communication between the two metal centres is often observed.

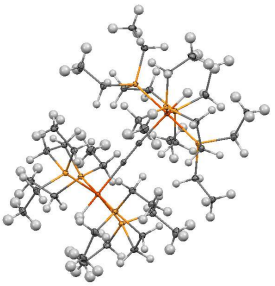


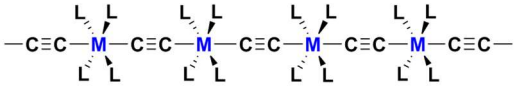


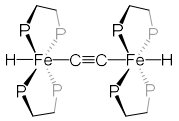
The majority of alkyne-bridged organometallic polymers use linear aromatic spacer units as the bridge between metal centres. We are interested in introducing bridges based on naphthalenes and other aromatic systems as well extending the oligomers to 2- and 3-dimensional networks.



We are also interested in systems where two metal centres are linked by just a single C≡C bridge. We recently discovered a straightforward route to an iron acetylide dimer so there is a proof of principle that the -M-C≡C-M- bridge can be made. We are looking for ways to extend the -M-C≡C-M-C≡C-M- chain to build up organometallic oligomers and polymers where multiple metal centres are bridged only by C≡C units.

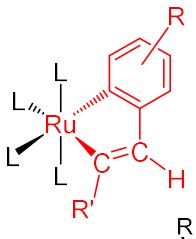




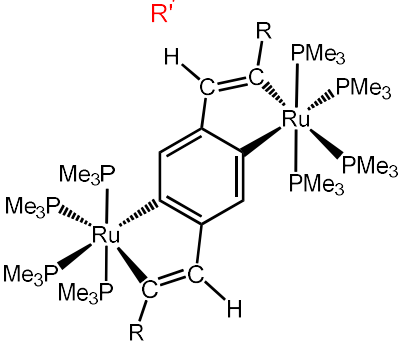


(b) Tuning the electronic properties of the metal centre in ruthenaindenes

The indene ring system has a benzene ring fused to a cyclopentene ring. Metalloindenes are cyclometallated ruthenium complexes where the ruthenium metal replaces one of the carbon atoms in the 5-membered ring of an indene molecule. In these compounds, the metal center is quite intimately embedded into the organic aromatic framework and we are examining the influence of substitution of the aromatic ring with strongly electron donating/withdrawing groups on the metal centre. Even though the metal centre is distant from the metal center, we know that the electronic properties of the substituents can be relayed effectively to the metal center.



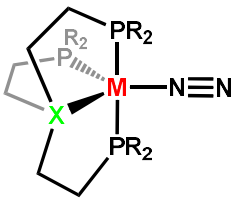
We are also exploring routes to di-metalloindecenes where the complex would contain two metal centres and here we expect to see strong metal-to-metal communication through the bridging aromatic ring.



(c) Metal complexes for Nitrogen fixation

The reduction of N_2 to NH_3 is one of the largest industrial processes in the world. We have recently developed a series of metal complexes with polydentate phosphine ligands [CP3 = $(R_2PCH_2CH_2)_3C^-$ and PP3 $(R_2PCH_2CH_2)_3P$]. When the metal is Fe or Ru, we know that the complexes bind and activate N_2 and allow the reduction of N_2 to NH_3.

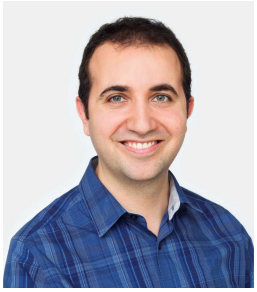
We are already exploring related complexes of Rh and Ir and we will expand the project to look at complexes of Co and Os to establish whether these metal complexes bind N_2 and how well they perform in producing ammonia from N_2.



X =P, C
M = Co, Os

Selected publications from the group:

1. Functionally Altered Ruthenaindenes with Electron-rich and Electron-poor substituents. Hsiu L. Li, Synøve Ø. Scottwell, James D. Watson, Timothy E. Elton, Hon C. Yu, Mohan Bhadbhade, Leslie D. Field, *Organometallics*, **2020**, *39*, 433−442. DOI 10.1021/acs.organomet.9b00788.
2. .Dinuclear Acetylide-bridged Ruthenium(II) Complexes with Non-aromatic Spacers. Surabhi Naik, Synøve Ø. Scottwell, Hsiu L. Li, Chanel F. Leong, Deanna M. D'Alessandro, Leslie D. Field, *Dalton Transactions*, **2020**, *49*, 2687–2695. DOI: 10.1039/C9DT04856A.
3. Reduction of Dinitrogen to Ammonia and Hydrazine on Low-Valent Ruthenium Complexes". Leslie D. Field, Hsiu L. Li, P. Manohari Abeysinghe, Mohan Bhadbhade, Scott J. Dalgarno, Ruaraidh D. McIntosh, Inorg Chem, 2019, 58, 1929−1934. DOI: 10.1021/acs.inorgchem.8b02850.
4. Fe(0)-Mediated Reductive Disproportionation of CO_2. Peter M. Jurd, Hsiu L. Li, Mohan Bhadbhade, Leslie D. Field, *Organometallics*, **2020,** *39*, 2011−2018. Published online at dx.doi.org/10.1021/acs.organomet.0c00175.



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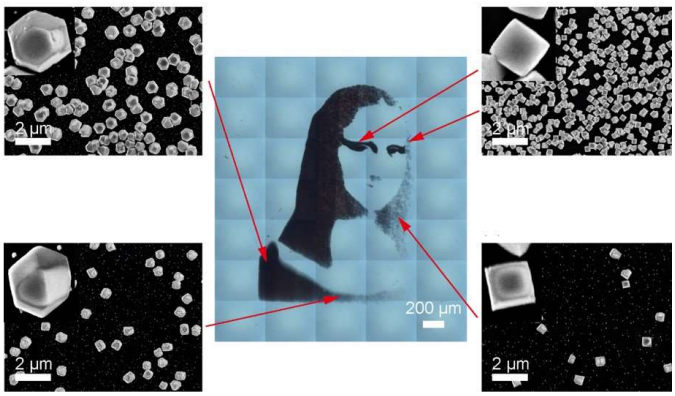
ELECTROCHEMICAL REACTIONS AT SEMICONDUCTORS

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:

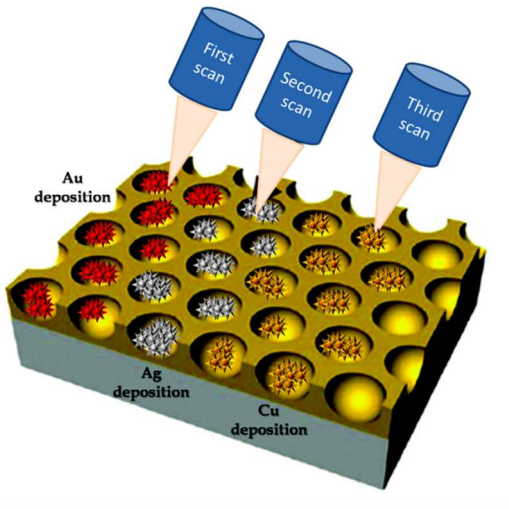
(a) Can we perform light-activated electrochemistry with improved spatial resolution? (in collaboration with Scientia Prof. Justin Gooding and Dr. Simone Ciampi / Curtin University)

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.



Cu_2O 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" muti-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)



Light-assisted electrodeposition of Au, Ag and Cu for sensors based on multi-metal nanoarrays.

This project intents 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.

[1] D. Polcari, P. Dauphin-Ducharme, J. Mauzeroll, "Scanning electrochemical microscopy: a comprehensive review of experimental parameters from 1989 to 2015", Chem. Rev. 116, 22, 1323, 2016.

[2] E. Cortón, S. R. Mikkelsen, "Electrochemical arrays for bioassay applications", "Trends in Bioelectroanalysis", F.-M. Matysik, Editor. Springer International Publishing, 103, 2017.

[3] M. H. Choudhury, S. Ciampi, Y. Yang, R. Tavallaie, Y. Zhu, L. Zarei, V. R. Gonçales, J. J. Gooding, "Connecting electrodes with light: one wire, many electrodes," Chem. Sci., vol. 6, no. 12, pp. 6769, 2015.

[4] Y. Yang, S. Ciampi, Y. Zhu, J.J. Gooding. Light-activated electrochemistry for the two-dimensional interrogation of electroactive regions on a monolithic surface with dramatically improved spatial resolution. J. Phys. Chem. C 120, 13032, 2016.

[5] Y.B. Vogel, V. R. Gonçales, J. J. Gooding, N. Darwish, S. Ciampi, "Cryptic nano inks: one-step electrochemical writing of Cu_2O nanocrystal patterns with hidden polyhedral signatures". Submitted.

[6] R. N. P. Colombo, D. F. S. Petri, S. I. Córdoba de Torresi, V. R. Gonçales, "Porous polymeric templates on ITO prepared by Breath Figure method for gold electrodeposition." Electrochim. Acta, 158, 187, 2015.

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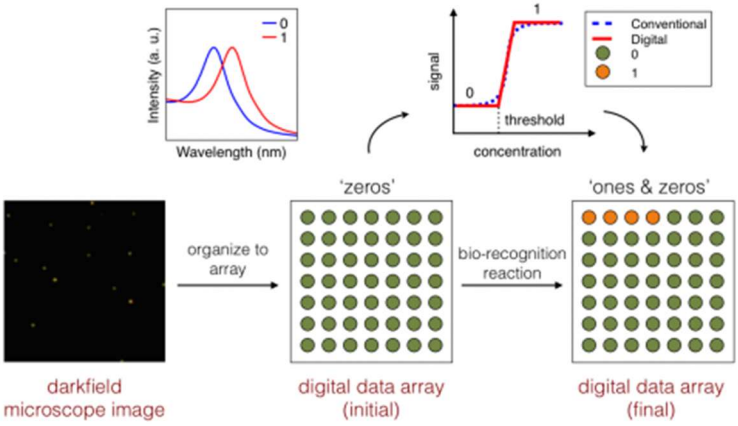
Australian Centre for NanoMedicine

SMART MATERIALS AND SURFACES

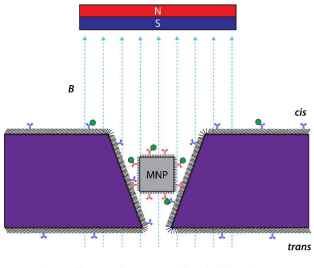
Our research group specializes in using self assembled monolayer or other surface modification technique to provide surfaces with unique functionality. The surfaces are the base upon which we build functional devices from nanscale component including polymer, protein, nanoparticles, and porous material. 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

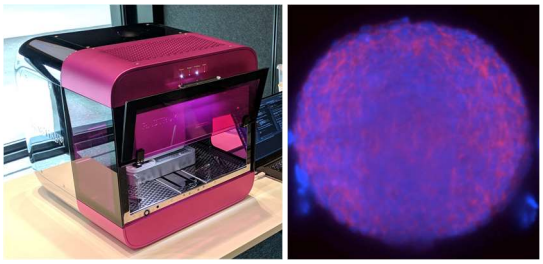


Specific antigen-antibody binding

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

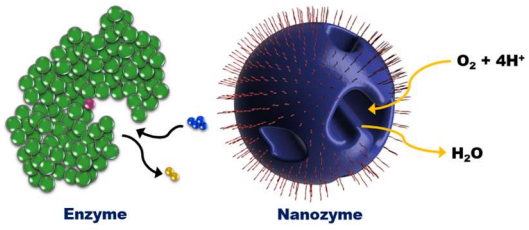
blockade sensor. In this system, antibody magnetic nanoparticles capture the analyte of interest and brign it to the nanopore. The nanopmodified nanoporesarticle then blocks the nanopore to give a single molecule measurement. An additional benefit is the nanopore blockade sensors can operate in complex biological fluids. This projest 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 fuels cells that mimic enzyme structure **(in collaboration with Professor Richard Tilley)**



Electrocatalysts are important is applications as broad as fuels 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 synthesize 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.

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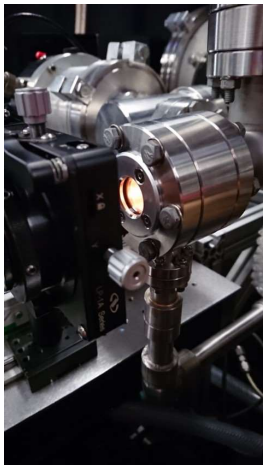
THE TRUE IMPACT OF FLUORINATED COMPOUNDS IN THE ATMOSPHERE

Use lasers to learn about the chemical reactions that occur after gas-phase fluorinated compounds absorb light. I am concerned about the true environmental fate of anthropogenic fluorinated compounds and have two projects looking at how light breaks down these molecules in the atmosphere. Use fundamental physical chemistry/chemical physics to address problems in atmospheric science.

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

Hydrofluorocarbons (HFCs) are the replacements to the chlorofluorocarbons (CFCs) and hydrochlorofluorocarbons (HCFCs). They have no ozone depletion potential yet still present an enormous risk to the environment as powerful global warming agents. These HFCs have a high infrared activity and long atmospheric lifetimes (decades to centuries) leading to global warming potentials (GWPs) up to 10s of 1000s of times worse than CO_2. The overall aim of both of these projects is to improve the underpinning science that is incorporated into atmospheric chemistry models so that humankind can (a) better understand the fate of long-lived compounds already emitted in large quantities and now phased out *i.e.* hydrofluorocarbons, and (b) understand the environmental risk of new compounds before they are emitted in large quantities.

(a) VUV Photodissociation of Hydrofluorocarbons



Hypothesis: Photodissociation in the upper atmosphere (mesosphere and higher) is a significant decomposition pathway for long-lived atmospheric fluorinated compounds.

The carbon-fluorine bond is the strongest single bond in organic chemistry, even strengthening neighbouring bonds, resulting in thermally-stable, volatile molecules that are chemically inert. Fluorocarbons are transparent to solar radiation through the stratosphere ($\lambda > 200$ nm), impervious to attack by atmospheric radicals, and insoluble in water. As these are the three dominant chemical sinks in atmospheric models, other pathways must become more important. This project hypothesises that photolysis by shorter wavelength light ($100 \text{ nm} \leq \lambda \leq 150$ nm) in the upper atmosphere might provide such a pathway.

My research group is one of few in the world that can produce laser light in the vacuum ultraviolet ($\lambda <$ 193 nm) for chemical dynamics experiments. This project will use lasers and velocity-mapped ion imaging to study the photodissociation of a series of hydrofluorocarbons to work towards a model of their photochemistry that may improve our understanding of their atmospheric lifetime.

(b) UV Photochemistry of Hydrofluoroolefins

Hypothesis: The GWP of a molecule's decomposition products needs to be considered when evaluating its GWP. Particularly for short-lived compounds celebrated as low GWP replacements for hydrofluorocarbons.

Current HFC replacements incorporate reactive chemical subunits (*e.g.* double bonds) that reduce their atmospheric lifetime to weeks. However, the most likely fluorine-containing end-products have a higher risk to the atmosphere than the compounds being replaced. This project aims to identify these products to assess the true atmospheric risk for emission of new fluorine-containing compounds.

Recent results from my group (in collaboration with Prof. Scott Kable's group) have revealed that the decomposition product of an important next generation refrigerant (HFO-1234ze or 1,3,3,3-tetrafluoropropene), with a GWP of zero, is removed from the atmosphere via photolysis to yield a significant quantity of the worst of the HFCs *i.e.* fluoroform (CHF_3) with a global warming potential ~13 000 times worse than CO_2. These results re-evaluate the 'effective' GWP to one in the 100s and also account for a detected and increasing, but otherwise unexplained, source of CHF_3 in the atmosphere.

This project will incorporate velocity-mapped ion imaging and Fourier-transform infrared (FT-IR) spectroscopy experiments, and possibly some computational chemistry, to elucidate the true atmospheric fate of these next generation refrigerants.

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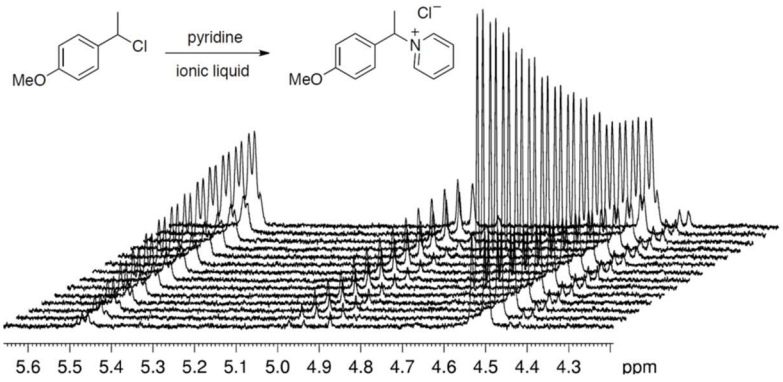
MECHANISTIC AND PHYSICAL ORGANIC CHEMISTRY

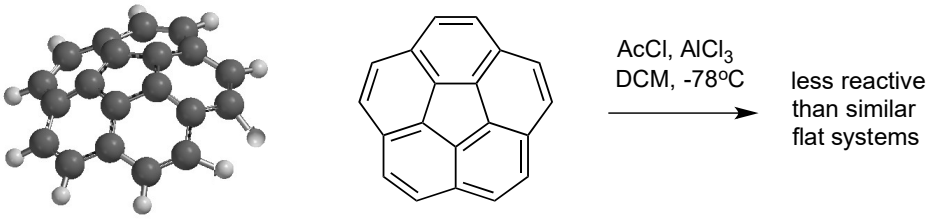
Our research is focussed on understanding how organic processes happen and what affects reaction outcomes. Particularly this encompasses examining how structural features in both the reagents themselves and the solvent used can change how a reaction proceeds. This knowledge can then be applied to a range 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 want[1] (in collaboration with Prof.'s Anna Croft and Christof Jäger, University of Nottingham, and Dr Ron Haines, 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!

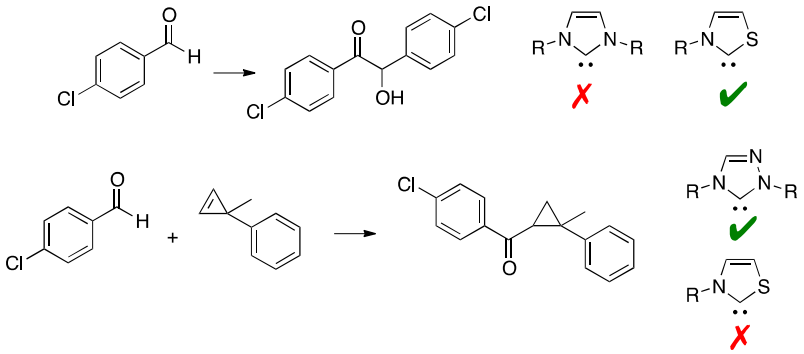
b) Non-planar aromatic hydrocarbons: different reactivity based on structure[2]



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.

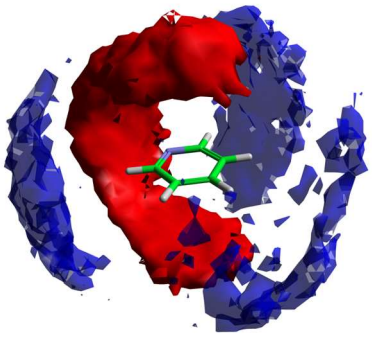
c) Catalysis using *N*-heterocyclic carbenes: understanding structure/activity relationships[3]



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.

d) Solvent-solute interactions in ionic liquids: can we design better solvents?[4] (in collaboration with Dr Ron Haines, UNSW; Prof.'s Anna Croft and Christof Jäger, University of Nottingham; and 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:

1. A. Gilbert *et al.*, *Org. Biomol. Chem.* **2020**, *1*, 5442; **2019**, *17*, 675 & 9336; K. S. Schaffarczyk McHale *et al.*, *ChemPlusChem*, **2019**, *84*, 465, 534 & 9243, **2018**, *83*, 1162; R. R. Hawker *et al.*, *Adv. Phys. Org. Chem.* **2018**, *52*, 49, *Org. Biomol. Chem.* **2018**, *16*, 3453 & *Org. Biomol. Chem.* **2017**, *15*, 6433.
2. S. R. D. George *et al.*, *Org. Biomol. Chem.* **2015**, *13*, 9035 & 10745 & *Polycycl. Arom. Compd.* **2016**, *36*, 897.
3. N. Konstandaras *et al.*, *Org. Biomol. Chem.* **2020**, *18*, 66 & 1910; *ChemistrySelect*, **2017**, *2*, 718; M. H. Dunn *et al.*, *J. Org. Chem.* **2017**, *82*, 7324.
4. R. R. Hawker *et al.*, *Chem. Commun.* **2018**, *54*, 2296 & *J. Phys. Org. Chem.* **2018**, *31*, e3862; J. J. Black *et al.*, *Phys. Chem. Chem. Phys.* **2018**, *20*, 16558; S. T. Keaveney *et al.*, *ChemPhysChem* **2018**, *19*, 3279; W. E. S. Hart *et al.*, *ChemPlusChem* **2018**, *53*, 348 & *Org. Biomol. Chem.* **2017**, *15*, 5556.

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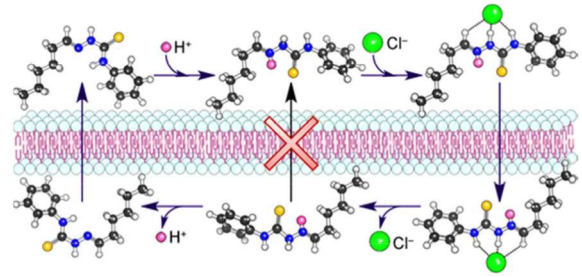
COMPUTATIONAL CHEMISTRY AND BIOMOLECULAR SIMULATIONS

We develop and apply computational chemistry methods to elucidate the mechanisms underlying many processes in synthesis and in biochemical systems (http://www.chemistry.unsw.edu.au/ho-group). 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 and supramolecular chemistry. We work closely with experimental groups (here at UNSW and from overseas) so projects can be tailored to include an experimental component if desired. The following outlines several representative projects but feel free to get in touch to discuss your interests. No background beyond 2nd year physical chemistry is assumed.

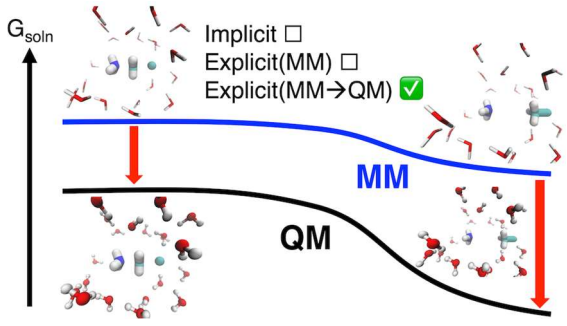
(a) Anionophores as novel anti-cancer agents

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 binding and transport process for several families of anionophores. In this project, you will learn how to carry out electronic structure calculations and classical molecular dynamics simulations to construct free energy profiles (fun stuff!). This project will help establish the molecular pre-requisites for anion transport that will facilitate the design of more effective drug candidates.



(b) Accurate prediction of reaction outcomes

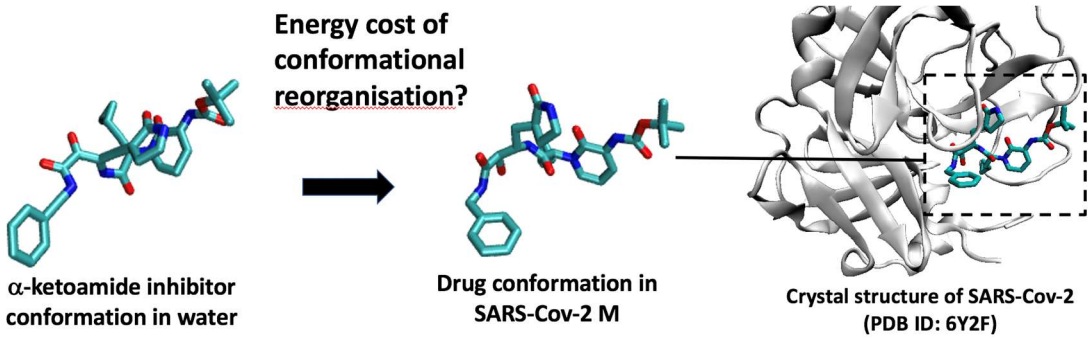
A significant milestone in computational chemistry is the development of highly accurate methods that can reliably predict the outcomes of gas phase reactions. Unfortunately, solution phase theoretical chemistry remains in a relatively primitive state where it is still very challenging to accurately predict the rate of even a simple S_N2 reaction in water! The goal of this project is to build on our recent work (e.g. *J. Phys. Chem.* **2019**, 123, 5580 and *Phys. Chem. Chem. Phys.* **2020**, 22, 3855) towards the systematic improvement of the description of solvent effects that



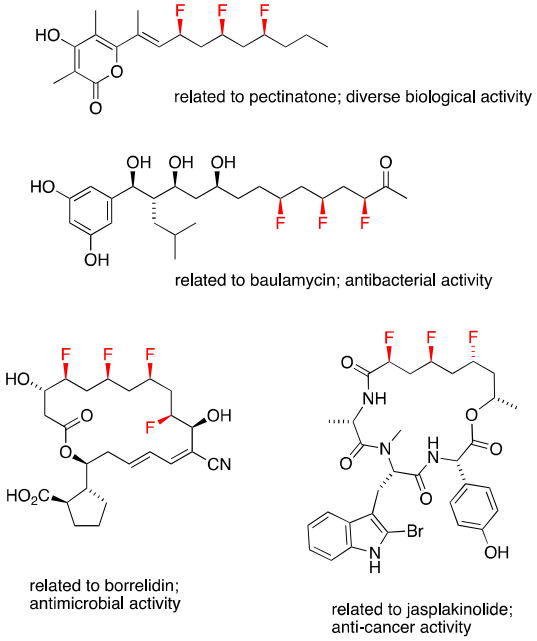
will enable chemists to reliably predict the yields and rates of chemical reactions. Specific areas include assessment of contemporary electronic structure methods to predict solvation energies and forces, and the development of efficient hybrid and fragmentation methods to accelerate their calculation. The initial goal is to focus on relatively simple organic reactions, e.g. S_N2 and Diels Alder reaction, before progressing to more complex multi-step reactions. The student will gain valuable skills in computational chemistry and programming to analyse large volumes of data.

(c) SARS-CoV-2: Understanding protein-ligand binding affinity

This project aims to understand how the conformational flexibility of a drug molecule may affect its binding affinity to the drug target. For example, the crystal structure of SARS-CoV-2 M^{pro} and its complex with an α-ketoamide inhibitor was recently reported (*Science* **2020**, 368, 409) and it is of interest to quantify the energetic cost associated with reorganisation of the drug from its native conformation into the shape it adopts when bound to the protein. This insight will be crucial for the design of improved drugs, e.g. through structural pre-organisation (see project (d)). It will also be valuable for improving predictions made by docking programs. The project will involve the development and application of computational tools to efficiently search the conformational space of large flexible drug molecules.



(d) Computer-aided design of fluorinated bioactive molecules (with A/Prof Luke Hunter)



Fluorination is often used by medicinal chemists to impart structural rigidity and/or tune the lipophilicity of drug molecules. This project will use computational techniques (e.g. docking, quantum chemical and molecular dynamics 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 on the left. There will also be an opportunity in this project to validate some of the computational predictions through synthesis.

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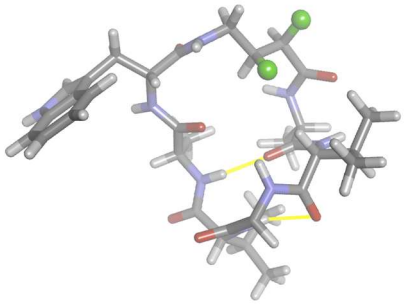
FLUORINE IN MEDICINAL AND ORGANIC CHEMISTRY

- 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:

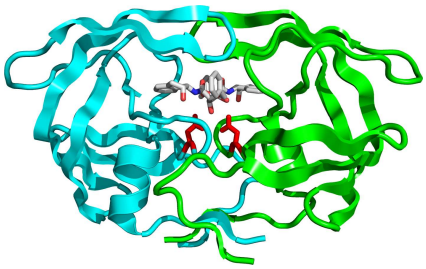
(a) Fine-tuning the shapes of cyclic peptides



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

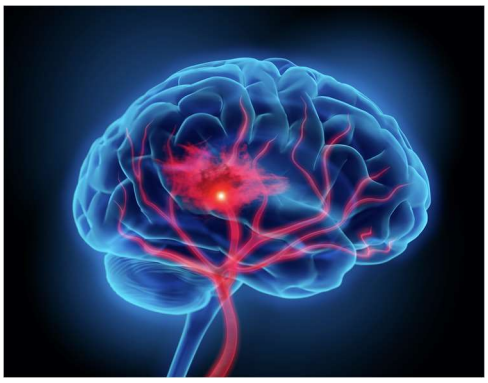
(b) Next-generation enzyme inhibitors



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.

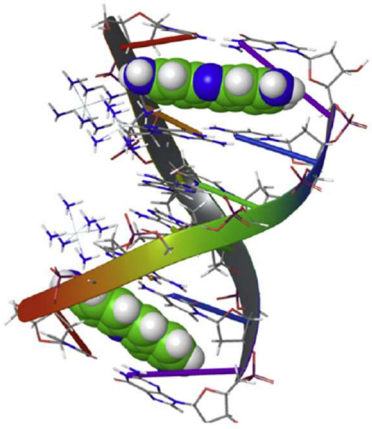
Collaborator: Dr Nicole Jones, A/Prof Renate Griffith

(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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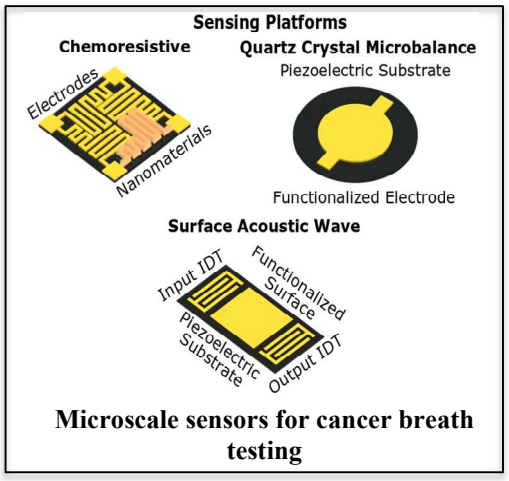
PORTABLE DEVICES FOR CHEMICAL ANALYSIS

I am an ARC DECRA Fellow in UNSW's School of Chemistry, collaborating closely with A/Prof. Alex Donald. My current research is focused on the development of portable chemical separations and detection devices, which can be utilized in a range of important applications such as air and water quality monitoring and non-invasive disease diagnosis.

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

(a) Microscale gas sensors for cancer breath testing

The diagnosis of cancer in an early stage can significantly improve disease prognosis. The early diagnosis of cancer is a significant challenge because such diseases are initially asymptomatic. Typically, cancer cells are diagnosed by a biopsy after an initial screen that is performed by either magnetic resonance imaging, computed tomography, positron emission tomography, X-ray imaging, mammography, colonoscopy and/or blood tests. These methods are typically not suitable for early-stage diagnosis. Thus, the development of non-invasive methods for the diagnosis of early stage cancer is of fundamental importance to improving patient outcomes.



Microscale sensors for cancer breath testing

In this context, the detection of volatile biomarkers from human exhaled breath to diagnose various cancer types has been an area of intense, recent research effort. Many volatile, semivolatile and non-volatile compounds may exist in such samples that are associated with various biochemical and metabolic processes. The growth of cancerous cells can have effects on these biochemical processes and change the chemical composition of the host, including at remarkably early precancerous disease stages. By measuring the VOC profiles, evidence from clinical trials suggest that the early detection of different types of cancer is feasible.

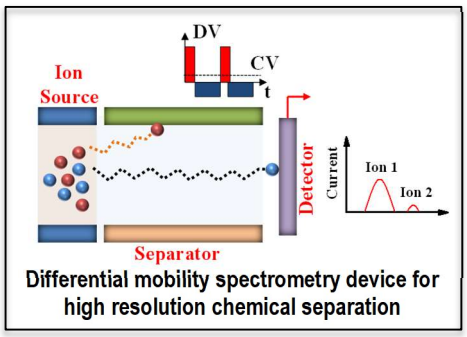
Even though commonly used gas/liquid chromatography and mass spectrometry-based methods allow universal chemical analysis with high sensitivity, they are not suitable for point-of-care diagnostics owing to their bulky size, rigorous sample pre-treatment requirement and long analysis time. Thus, recent research has focused on developing portable chemical sensors such as chemo-resistive, surface acoustic wave and quartz crystal microbalance-based devices to enable point-of-care diagnostics by profiling cancer related VOCs. In this project, you will study such portable chemical sensors that can potentially make a significant impact in cancer diagnosis and thus in human lives.

Under this approach, cancer is typically detected by comparing the concentration levels of many different VOCs (or a VOC 'fingerprint') between samples from cancerous and healthy subjects. Thus, a

multi-sensor approach is typically employed in which a group of semi-selective sensors are integrated in an array, which is sometimes referred to as an electronic nose (eNose). Upon exposure to the targeted VOCs, individual sensors within the broader array can respond differently to different types of cancer-related volatile compounds (e.g. aldehydes, ketones, alkanes, and organic acids) and thus, a fingerprint for a given VOC mixture can be obtained. Normally, an array of cross-reactive sensors is utilized where each sensor is coated with a different material that influences the extent that the particular sensor responds to different types of analytes. Thus, each analyte type gives a distinctive pattern response from the array. The major advantages of such sensors are their portability, fast analysis times, low detection limits, often simple fabrication procedures, economical cost and ease of use. By working in this project, you will learn the process of device development and operation that includes photolithography, silicon processing, nanomaterials development and sensing system setup.

(b) Differential ion mobility spectrometry for separation of gas-phase ions

Rapid and accurate separation between the gas-phase ions with close sizes, molecular shapes and charges is highly important for different biological, environmental and security applications. For example, chiral recognition of amino acid enantiomers such as tryptophan and phenylalanine is important for drug development. The analysis of persistent organic pollutants, such as perfluoroalkyl substances is required to ensure water quality.



Differential mobility spectrometry device for high resolution chemical separation

Among various methods used for gas-phase ion separation, ion mobility spectrometry (IMS) is particularly promising as IMS can be integrated with mass spectrometry (MS) to readily reduce background noise while analysing complex samples and can eliminate the requirement of chromatographic system, which needs long analysis time and rigorous sample pre-treatment. In this project, you will develop and investigate the performance of a more powerful and a new class of IMS device, known as differential ion mobility spectrometry (DMS), for various chemical analysis.

In a conventional IMS, gaseous ions can be rapidly separated and detected based on the drift velocity of ions through a buffer gas under a weak electric field. However, under the operating electric field of IMS, the mobilities of ions are independent of electric field and are separated based only on their drift velocity in a given carrier gas. Many types of ions may have similar mobility in a given carrier gas and therefore cannot be resolved with IMS. This ultimately leads to false positives and reduce confidence in ion assignment.

To overcome such limitations of conventional IMS, a relatively new method that has been recently developed is differential mobility spectrometry (DMS). DMS instruments separate and detect gas phase ions based on the use of high electric fields and thus, they can have a higher resolving power than conventional IMS devices. In our lab, we have both macro and microscale DMS devices that you can use to analyse various types of important ions such as amino acids, perfluoro compounds and protonation isomers. You will also have the opportunity to be involved in the design and development novel DMS devices that will significantly improve the performance of currently available DMS devices.

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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:

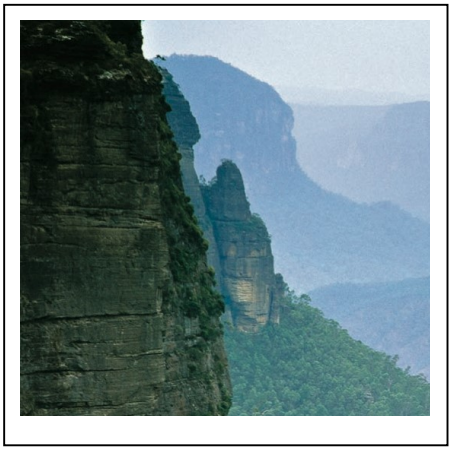
(a) Weird chemistry – reactions that just don't go where they should. (Collaborators: Meredith Jordan, Sydney Univ.)

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:

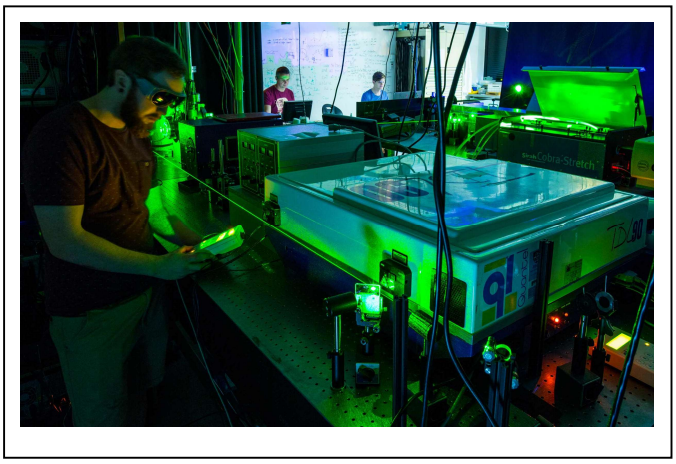


Dihydrogen (H_2) in the atmosphere is a trace species with a concentration of around 500 parts per billion. As a long-lived species (half-life ~ 2 years), it has been considered to be relatively unimportant. However, atmospheric models cannot account for observed amount of H_2. Modelers believe that there is a missing source of H_2 that is photochemical in nature. The possibility that H_2 will find broad application as a "green fuel" (there are already H_2 cars) means that large-scale leakage of H_2 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 H_2 before we reach this point. In recent research, we have discovered that many carbonyls are a source of H_2 when exposed to ultraviolet light. In this Honours project, you will make measurements of H_2 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 (CO_2). 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 (CO_2 and H_2O) 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 H_2O 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.

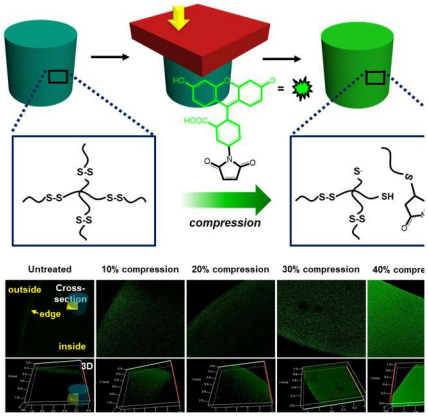

Fig. 1. Compression ruptures disulfides for subsequent reaction with acceptor

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

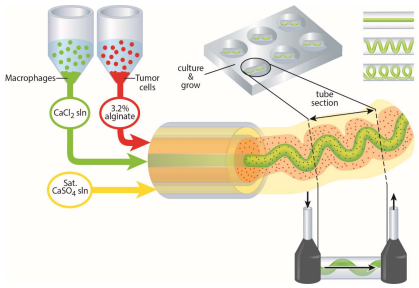

Fig. 2. Extrusion of cell-laden chemically modified alginate (*Adv. Mater., 2015*)

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

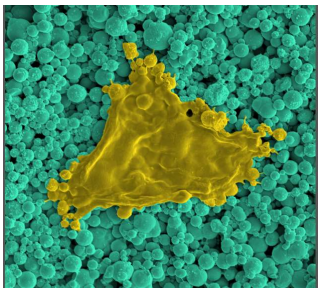

Fig. 3. Cancer cell adherent to iron particles in a hydrogel (*Adv. Health. Mater.,* 2016)

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 involves: 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)

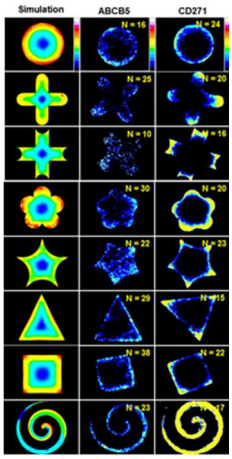

Fig. 4. Interfacial curvature will guide the activation of a stem-like state (*Nat. Mater.*, 2016)

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.

Junmin Lee, Meredith N. Silberstein, Amr A. Abdeen, Sang Yup Kim, and Kristopher A. Kilian, Mechanochemical functionalization of disulfide linked hydrogels, Materials Horizons, 2016, 3, 447-451

Joshua M. Grolman, Douglas Zhang, Andrew M. Smith, Jeffrey S. Moore, and Kristopher A. Kilian, Rapid 3D extrusion of synthetic tumor microenvironments, Advanced Materials, 2015, 27 (37), 5512-5517

Amr A. Abdeen, Junmin Lee, N. Ashwin Bharadwaj, Randy H. Ewoldt, and Kristopher A. Kilian, Magnetoactive hydrogels for temporal modulation of stem cell activity, Advanced Healthcare Materials, 2016, 5 (19), 2536-2544.

Junmin Lee, Amr A. Abdeen, Kathryn L. Wycislo, Timothy M. Fan, and Kristopher A. Kilian, Interfacial geometry dictates cancer cell tumorigenicity, Nature Materials, 2016, 15, 856-862.

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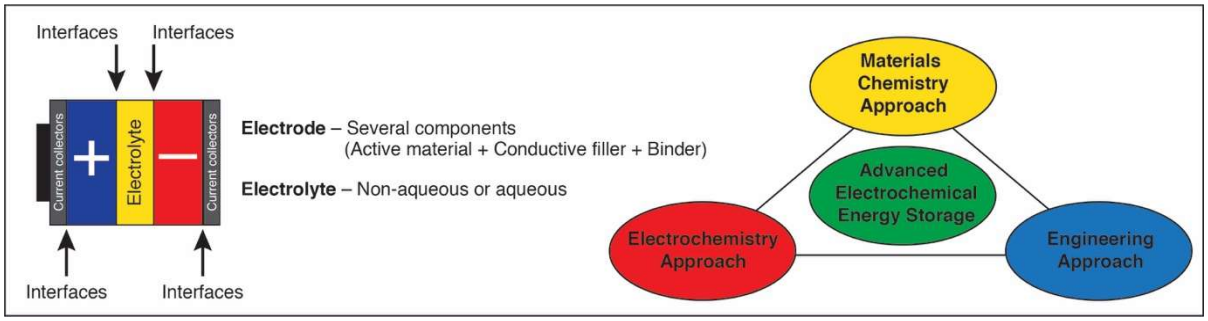
ADVANCED ENERGY MATERIALS CHEMISTRY

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 approach is based on combining synthetic chemistry, electrochemistry, and materials science principles to develop advanced energy storage devices, in particular, rechargeable batteries. Additionally, we expect 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) Designing rechargeable Al-ion batteries (in collaboration with Dr. Neeraj Sharma)

Aluminium is the third most abundant element in the Earth's crust. 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.

Recently, we demonstrated[6] one of the first rechargeable Al-ion batteries. Our approach was the utilisation of the triangular macrocyclic compound, which form layered superstructures resulting in the reversible insertion and extraction of an aluminium complex. This architecture exhibits an outstanding electrochemical performance along with superior cycle life.

The overarching goal of this Honour project 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[5], the redox-active compounds based rechargeable Al-ion batteries could provide a promising starting point for developing affordable large-scale energy storage applications.

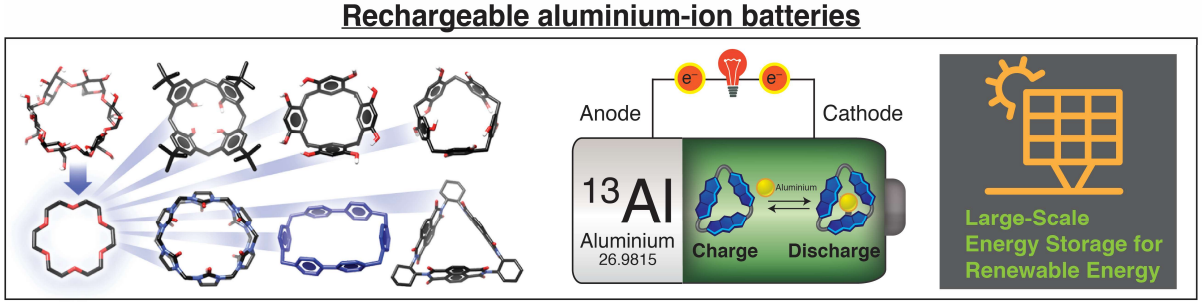


Figure 1. Graphical representation of the macrocyclic building blocks into nano-channels.

(b) Bio-inspired chemistry for rechargeable batteries

We have found that the mussel-inspired catechol functional group is a useful moiety for enhanced cycle lives in Lithium–Sulfur battery configuration. The wet-adhesive property originating from the catechol groups turned out to play a decisive role for increasing the cycle life, particularly in an environment where the electrode films are in direct contact with wet liquid electrolytes, similarly to mussel feet with extraordinary adhesion capabilities during the contacts with wet objects in the sea. In this project, we will design a polydopamine coated electrode-active materials, in order to increase the electrochemical performances of the next-generation battery system.

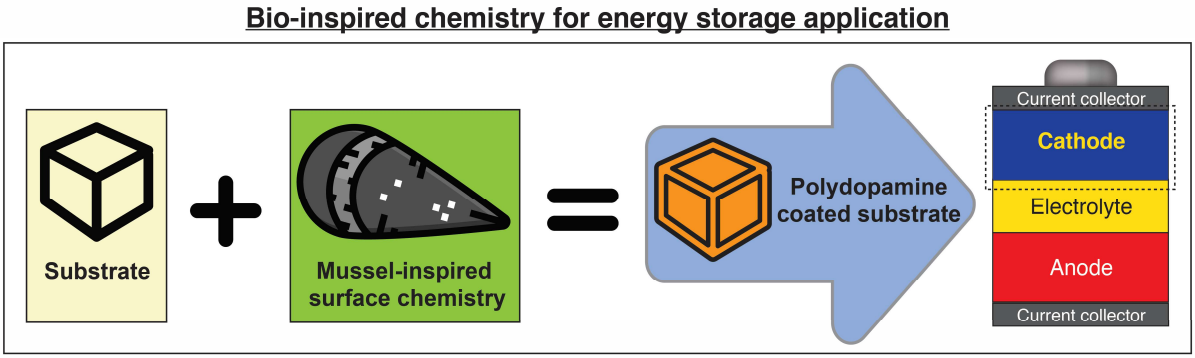


Figure 2. Utilisation of mussel-inspired polydopamine coating for the energy storage application.

1. Huggins R. *Advanced batteries: Materials science aspects.* Springer Science & Business Media, 2008.
2. Armand M. & Tarascon J.-M. Building better batteries. *Nature* **451,** 652–657 (2008).
3. Choi J. W. & Aurbach D. Promise and reality of post-lithium-ion batteries with high energy densities. *Nat. Rev. Mater.* **1,** 16013 (2016).
4. Elia G. A., *et al.* An overview and future perspectives of aluminum batteries. *Adv. Mater.* **28,** 7564–7579 (2016).
5. Kim D. J., *et al.* Redox-active macrocycles for organic rechargeable batteries. *J. Am. Chem. Soc.* **139,** 6635–6643 (2017).
6. Kim D. J., *et al.* Rechargeable aluminium organic batteries. *Nat. Energy* **4,** 51-59 (2019).

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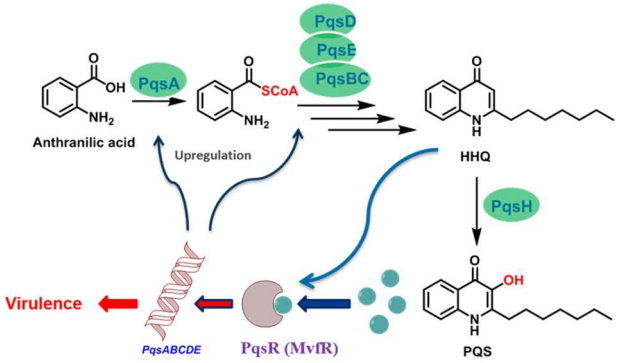
SYNTHETIC ORGANIC AND MEDICINAL CHEMISTRY

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.

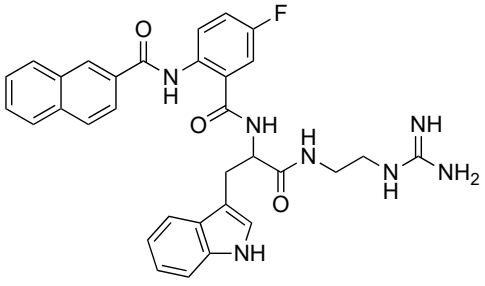
(a) DESIGN AND SYNTHESIS OF NOVEL ANTIMICROBIAL AGENTS

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. *Pseudomonas* quinolone system (PQS).

New scaffolds for antimicrobial discovery



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.

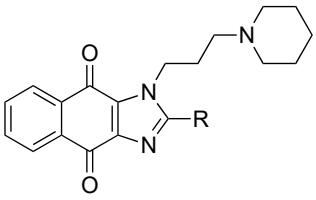
Inhibitors of Bacterial Transcription Initiation

(in collaboration with A/Prof. Renate Griffith, UNSW and Prof. Peter Lewis, University of Newcastle)

The enzyme RNA polymerase (RNAP) that transcribes DNA into RNA is highly conserved across species. However, the factors that regulate the activity of RNAP are target-specific. Therefore, the unique interaction of sigma factors with RNAP in bacteria represents an ideal target for the development of small molecules that can specifically inhibit this interaction[3]. In this project new molecules that target these essential protein-protein interactions will be rationally designed and synthesized, and evaluated for their antimicrobial efficacy. These new small molecules would represent lead compounds for the development of new antibiotics.

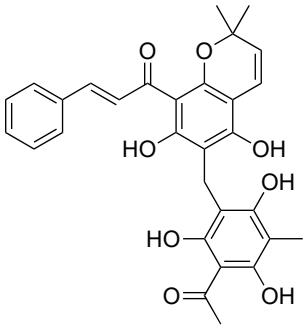
(b) DEVELOPING ANTICANCER COMPOUNDS THAT ACTIVATE GLUCOSE OXIATION

(in collaboration with Dr Frances Byrne and A/Prof 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 (CO_2) 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) DESIGN AND SYNTHESIS OF NOVEL HETEROCYCLIC SYSTEMS



Flavones and isoflavones are two structurally related large and diverse groups of natural compounds with broad spectra of biological activities including antioxidant, anticancer, antiviral and anti-inflammatory properties. They are recognized as “privileged” medicinal chemistry molecular frameworks because they are commonly found in biologically active compounds that show drug-like characteristics. Rottlerin is a flavonoid isolated from the fruits of a medicinal plant, *Malloutus philippensis*. Our group has reported the successful synthesis of rottlerin via the acid-catalyzed reaction of 5,7,8-trimethoxyflavene. A number of projects are available in this area focussing on the design and synthesis of new azaflavone analogues of flavones and isoflavones in which the ring oxygen atoms are replaced by a nitrogen atom.

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COMPUTATIONAL MATERIALS SCIENCE AND CHEMISTRY FOR SUSTAINABILITY APPLICATIONS

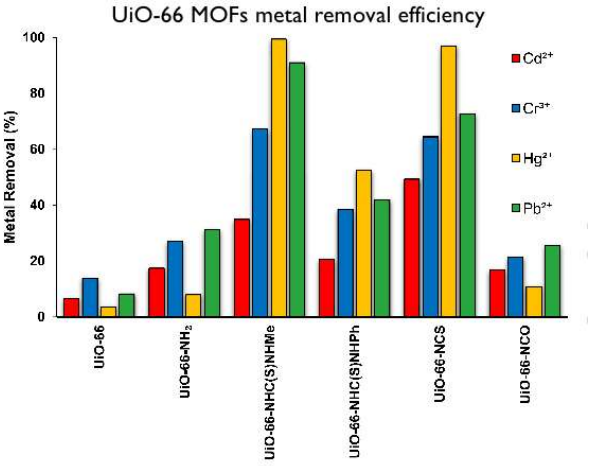
Computer simulations are an essential tool to make high-impact discoveries in fields that are crucial to our sustainable future. In general, these types of simulations allow us to calculate properties of molecules and materials at the atomic scale, which can be too difficult to be measured by experiments. This information can be used to unravel the fundamental chemistry features of a system responsible for promising experimental observations and thus rationally guide experimental efforts towards optimizing those features for the application of interest.

Research in my group focuses on using computer simulations to tackle a variety of sustainability issues, including the development of new renewable energy and water purification technologies. Additionally, **I am eager to explore new application areas for computational chemistry, such as art conservation** (see example project on the next page). Working on these projects will allow you to acquire/strengthen knowledge and skills in a variety of fields in chemistry, physics, and computer programming. Furthermore, most of the projects involve close collaboration with groups at UNSW and overseas (United States and Europe). Please don't hesitate to contact me to discuss possible projects in more details and/or your research interests. No prior knowledge of programming or computational chemistry is required.

Some of the projects currently available are:

(a) Computational Design of Metal-Organic Frameworks for Heavy Metal Removal from Water

Access to clean water has been recognized as an essential human right by the United Nations. However, water contamination issues still exist and often render drinking water unsafe even in well developed countries. Developing cost-effective and efficient materials for water treatment is necessary to ensure access to clean water for all. Heavy metals are particularly hazardous contaminants because they pose serious risks to human health and can enter our water supply in multiple ways. The scientific community is thus searching for new materials that are both cost-effective and selective for heavy metals.



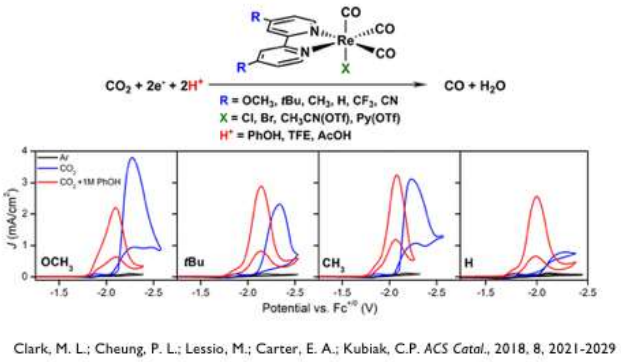
Saleem, H.; Rafique, U.; Davies, R. P. *Microporous Mesoporous Mater.* 2016, 221, 238–244

In this project, we will use computational chemistry to aid the development of new materials based on metal-organic frameworks (MOFs) for the adsorptive removal of heavy metals from water. MOFs are very promising for adsorption-based water treatment technologies due to their extremely high surface area, the possibility to tune their selectivity by functionalizing their surface, and the possibility to alter their pore size by choosing different building

units. Indeed, MOFs belonging to the UiO-66 family have already been shown to possess a much greater adsorption capacity for heavy metals than commercially available adsorbents. In this project, we will elucidate the adsorption mechanism at work in these MOFs using computer simulations and use the acquired knowledge to design improved systems.

(b) Carbon Dioxide Reduction Using Transition-Metal Complexes

CO_2 conversion into liquid fuels is a promising avenue towards efficient electrical energy storage and at the same time reduction of the CO_2 concentration in our atmosphere. Transition metal complexes have been shown to be capable electrocatalysts for the conversion of CO_2 into useful products. However, they typically require large energy inputs to reach their active catalyst state and are often made of rare and expensive metals.

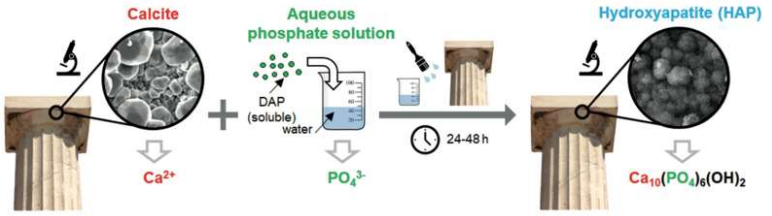


Clark, M. L.; Cheung, P. L.; Lessio, M.; Carter, E. A.; Kubiak, C.P. *ACS Catal.*, 2018, 8, 2021-2029

In this project we will use computational tools to study how the performance of these catalysts is affected when using more abundant metals, with the aim of designing cheaper and more effective catalysts. Additionally, we will also attempt to optimize the performance of these catalysts by studying the effect of changing the ligands and counterions. Overall we expect the results of this project to guide experimental efforts towards the synthesis of improved and more cost-effective catalysts for CO_2 reduction.

(c) Computational Chemistry Meets Art Conservation: Design of Improved Surface Protective Treatments for Marble

Computer simulations are an established tool in the investigation of solid/liquid interfaces in many different fields ranging from materials science to biological applications. Solid/liquid interfaces are often the focus of art conservation efforts as solid artefacts are often exposed to harmful liquids. In spite of its great potential, the application of computational chemistry in the field of art conservation is still extremely limited.



Sassoni, E. *Materials* 2018, *11*, 557

In this project, we will use computational tools to investigate the chemical mechanism behind an innovative treatment for the protection of marble artefacts exposed to water. We will then use the acquired knowledge to develop improved protective treatments in close collaboration with conservation scientists at the University of Bologna, Italy.

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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

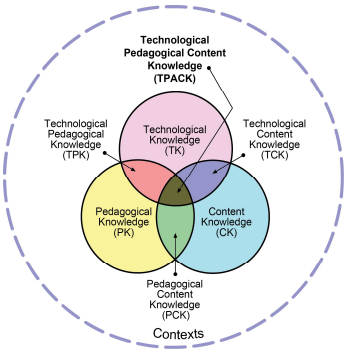
The world is currently facing unprecedented challenges which are affecting all facets of life on earth. Climate change, Sustainability and the need for Renewable energy sources and storage are challenges which have chemistry at their core. A recent article in Nature Reviews Chemistry[1] served as a call 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.

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

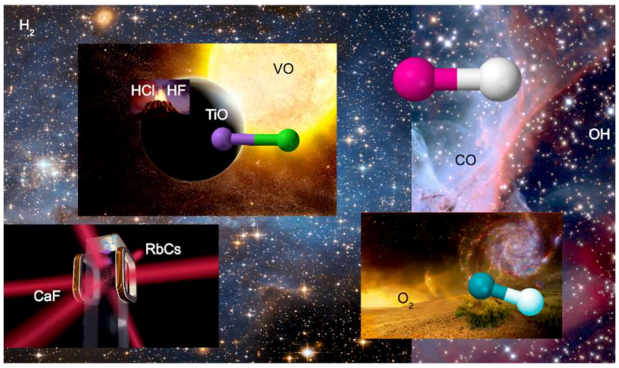


Keywords: *Digital Literacy, PCK, TPACK, Online learning, Blended Learning*

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[2].

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.

1. Mahaffy, P. G., Krief, A., Hopf, H., Mehta, G. & Matlin, S. A. Reorienting chemistry education through systems thinking. *Nature Reviews Chemistry* (2018). doi:10.1038/s41570-018-0126
2. Koehler, M. J., & Mishra, P. (2009). What is technological pedagogical content knowledge? *Contemporary Issues in Technology and Teacher Education, 9*(1), 60-70.

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EXPLORING QUANTUM CHEMISTRY & MOLECULAR PHYSICS

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 projects with customisable amounts of chemistry, physics, mathematics, programming, data science and education/outreach.

During a research 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 and quantum chemistry programs, data science, data presentation, debugging and, perhaps most importantly, "Googling".

My major research focus is method development for and applications of computational molecular spectroscopy. As an example of the projects I offer within this area:

Life on Venus? A case of mistaken identity, new chemistry or new biology?

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

The recent detection of phosphine on Venus relied on just one spectral line. How do we know it is phosphine? How might phosphine be produced – chemically, geologically or biologically? What other molecules would we expect to co-exist? New theories will be emerging regularly to try to explain phosphine in Venus – perhaps here at the UNSW Astrobiology centre. These theories will predict related phosphorus containing molecules.

This project will focus on producing spectral data to enable astronomers to test these new predictions.

How to model your NMR spectra: What basis set and level of theory should you use?

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 structural information the spectra provides. Accurate computational chemistry calculations can assist with both these tasks for difficult cases like fluorine-containing compounds. However, existing calculations often use sub-optimal basis sets that do not adequately describe the electron core region, with scaling factors used to fix these inadequacies.

In this project, you will explore the quality of NMR spectral predictions using existing and novel basis sets used alongside popular density functional approximations.

Looking for New Physics using Spectroscopy

Keywords: Beyond Standard Model, Computational Chemistry, Rovibronic Spectroscopy

New theories of physics that attempt to unify gravity and the standard model of matter often predict variation in the proton-to-electron mass ratio. This variation can be measured astrophysically through transitions in molecules. CP, SiN and SiP are as yet unexplored astrophysical diatomic molecules that have the potential to be used as molecular probes of proton-to-electron mass variation.

In this project, you will be creating a rovibronic line list of the energy levels and transition intensities for these molecules using sophisticated quantum chemistry packages and available experimental data. Beyond the primary objective, this data will also be used to look for these molecules in other astrophysical bodies such as stars, planets and exoplanets; the presence of unusual molecules give essential knowledge about the chemistry and physics of their environment (e.g. phosphine on Venus).

Beyond this main body of work, some of my research projects at the moment include:

Why is B3LYP/6-31G* still so popular?

Keywords: Data extraction, Change theory, Computational chemistry, Qualitative research, Data analysis

B3LYP/6-31G* was the state of the art quantum chemistry method … around the year 2000. Yet the widespread availability of better model chemistries (as benchmarked extensively), this older theory is still used extensively, especially for organic chemistry applications.

In this project, we will investigate the choices users make: what, how & why. This will be correlated to data on how method developers try to reach potential users. The data will be collected via interviews, surveys and parsing online data sources and analysed using the lens of change theory.

Exploring NSW laws for Illegal Drug Analogues using Cheminformatics (collaboration with Brynn Hibbert).

Keywords: Python, Application, Cheminformatics, Algorithm Design

Replacing a hydrogen with a fluorine atom often does little to affect the biological function of a molecule, so lawmakers need to ensure that molecules that are similar to illegal drugs are also illegal. But are the current laws too widespread – most critically, do they limit potential pharmaceutical medicines? In this project, you will enumerate illegall drug analogues and consider the implications of this law.

Developing a new technique for literature reviews (collaboration with Clarivate Analytics).

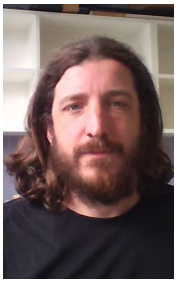
Keywords: Algorithm Development, Literature Review, Commercial Applications

Good quality literature reviews are crucial for good science, but take time. Here, you will help develop an algorithm under a non-disclosure agreement with the team responsible for Web of Science.

Evaluating SciX research-teaching-outreach project (collaboration with Shannan Maisey).

Keywords: Citizen Science, Education/Outreach/Teaching, Science Education, Evaluation

NSW Year 12 students have the opportunity to engage with a one-unit Science Extension course, where they pursue an independent research project ideally in collaboration with university researchers. At UNSW, we have developed SciX as a pathway to ensure equitable and widespread access to university research and researchers, and want your help in establishing and evaluating this programme's effect on the PhD student mentors, high school student researchers and other stakeholders.



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PROBING ATMOSPHERIC REACTIONS WITH MICROWAVE SPECTROSCOPY

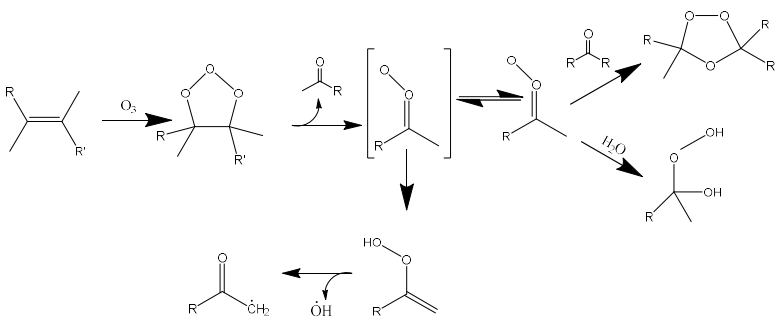
Chirped pulse Fourier Transform Microwave (CP-FTMW) Spectroscopy is a powerful new technique for rapidly acquiring rotational spectra. This allows for the precise determination of the 3D structure of gas phase molecules. I am building up the only laboratory in the southern hemisphere with such an instrument. You can be involved in the construction, optimisation and use of this instrument.

Work in this laboratory is focused on atmospheric chemistry and can involve many different skills and techniques however a project can be tailored to fit the student's interests. In addition to the recording and analysis of microwave spectra projects may include programming, quantum chemical calculations, instrumental development and some synthetic chemistry depending on your interests.

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

(a) Step-by-step analysis of ozonolysis reactions

The reaction of ozone with hydrocarbons in the atmosphere is a highly complex process which leads to the production of many different species. This reaction can branch to form different compounds depending on the starting conditions and structure of reactants. The 3-D gas phase structure at each step of the reaction is crucial in the understanding the stability and reactivities of various compounds. You can use the new spectrometer to measure the microwave spectrum of atmospherically important molecules and monitor the reaction with ozone.

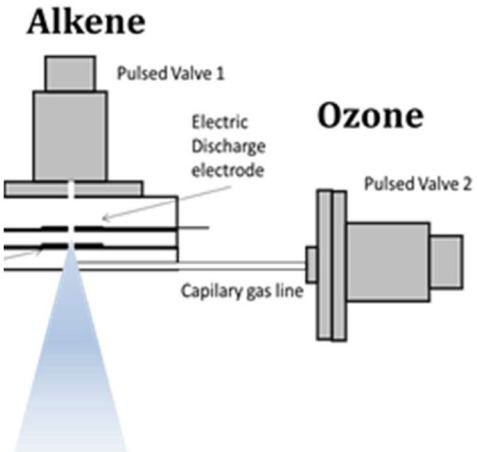


(b) Instrumental design and testing

Since this spectrometer is brand new there is the opportunity to build more than just chemicals. For example:

Design and 3-D printing of chemical reaction valves

Pulsed valves are widely used in spectroscopy to create cold molecules via supersonic expansion into a vacuum chamber. Here two such valves will be coupled together to mix two reactive chemicals and 'freeze' the reaction so that unstable or reactive compounds can be studied. 3D printing offers a rapid way to prototype different designs. You can design and test the performance of these valves to optimise them based on the production of certain molecules by monitoring their microwave spectra.



PROF. JONATHAN MORRIS

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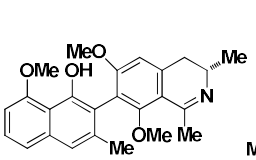
SYNTHETIC AND MEDICINAL CHEMISTRY

- 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.

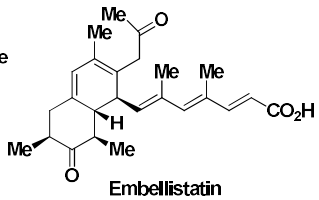
It would be great to work with Honours students on the following projects:

(a) Total Synthesis of Biologically Active Natural Products

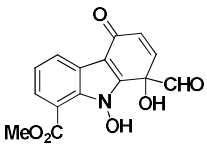
The development of efficient syntheses of biologically active natural products continues to be a major activity of the Morris group, with recent targets including ancistrotanzanine A, embellistatin and coproverdine. As syntheses of these targets are completed, work is initiated on their mode of action 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.



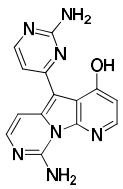
Ancistrotanzanine A



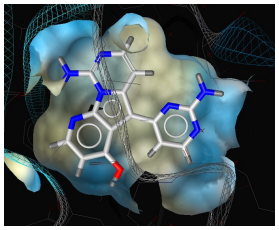
Embellistatin

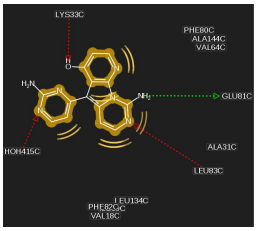


Coproverdine



Variolin B





(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

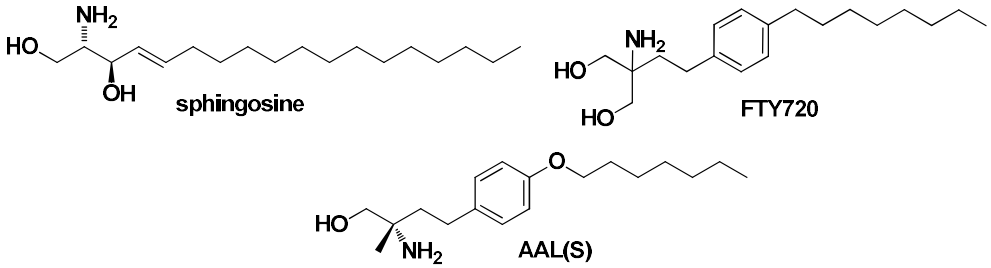
mediate the phosphorylation. This work originated from earlier work on the synthesis of a natural product. Variolin B is a member of a unique class of marine alkaloids isolated from an extremely rare Antarctic sponge. It is no longer available from its natural source. The Morris group have devised a 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)

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COORDINATION COMPLEX CHEMISTRY

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.

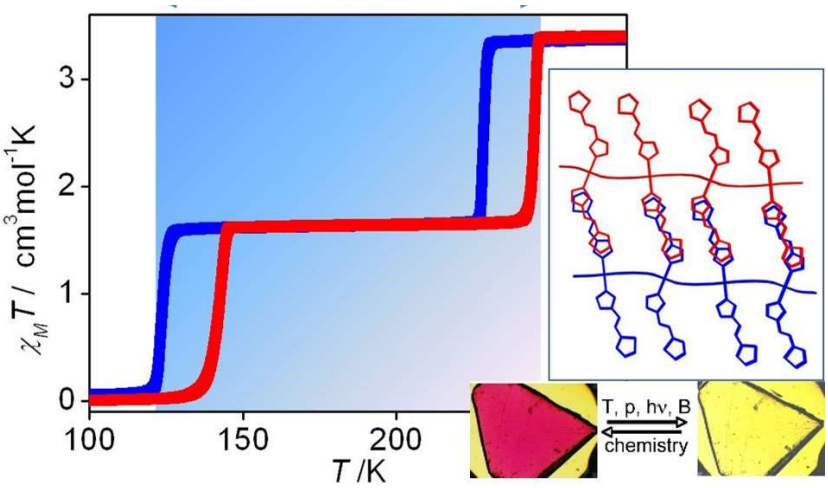
Skills you will learn:

- 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:

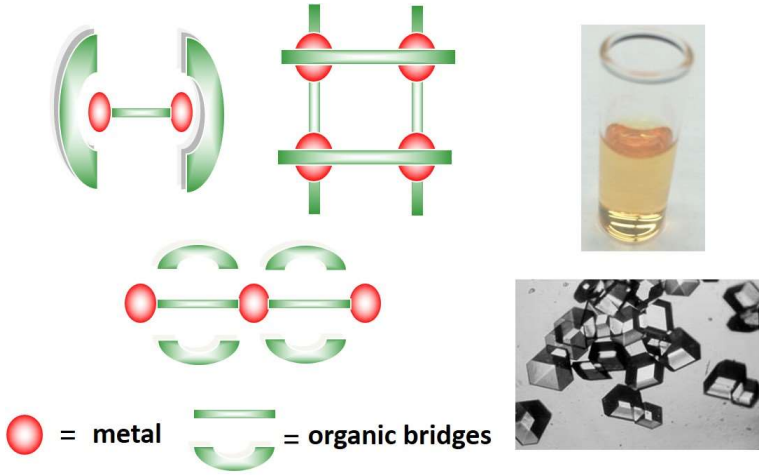
(a) Functional coordination polymers

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.



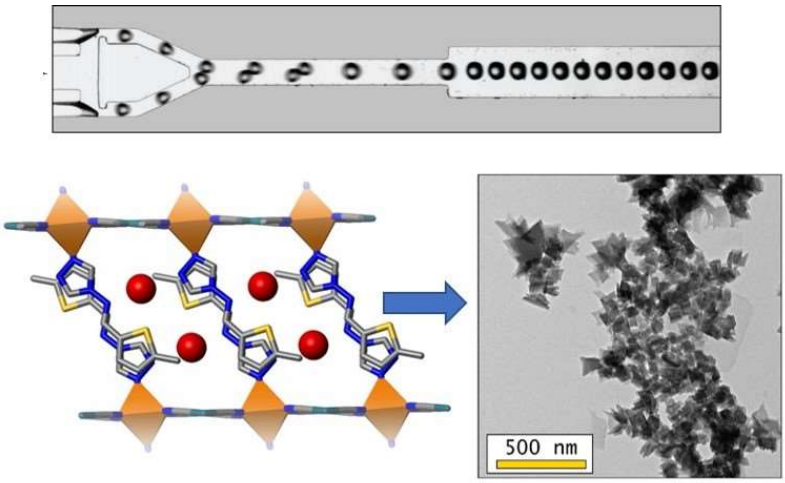
(b) Switchable square and cage complexes

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 d^{4-7} 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!).



(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.



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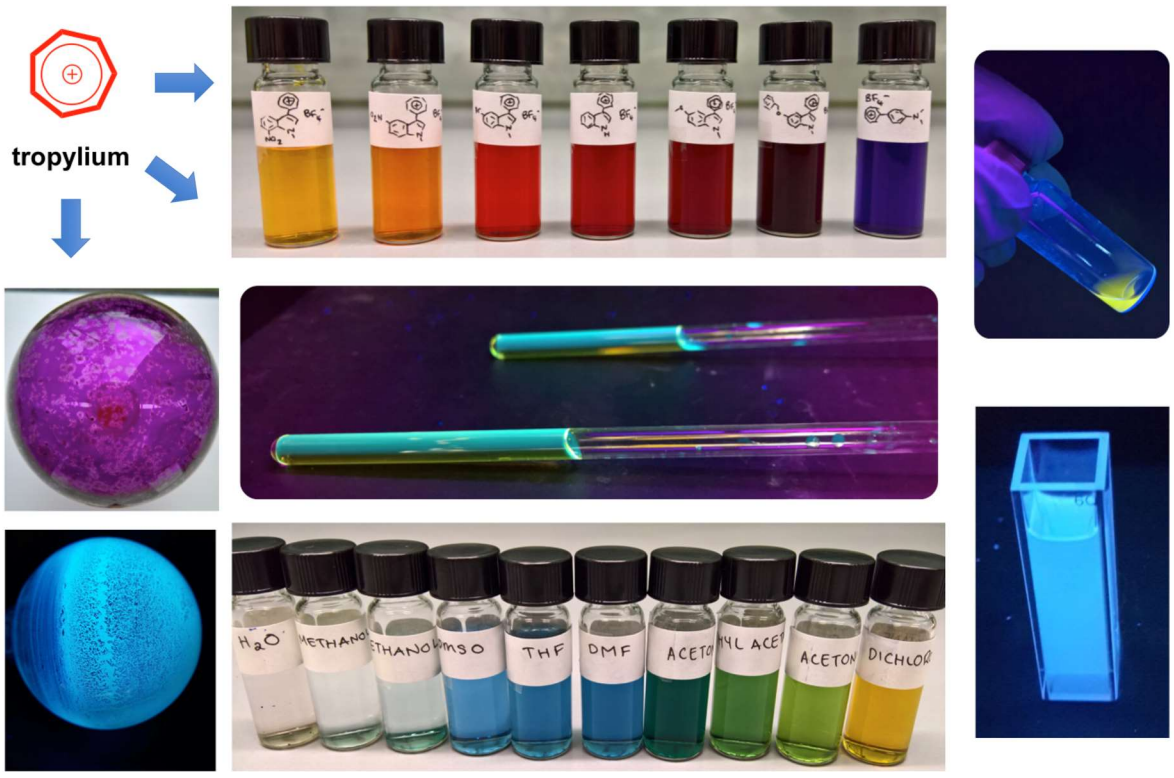
ORGANOCATALYSIS AND CHEMISTRY OF UNUSUAL MOLECULES

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

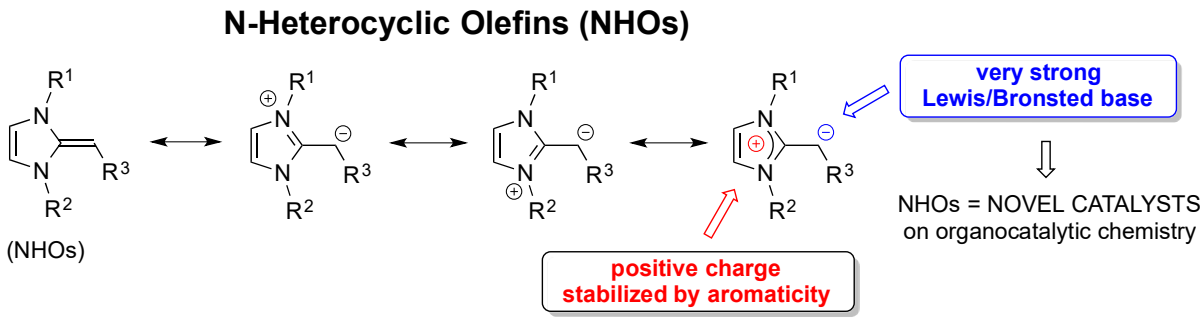
Tropylium ion is an unusual non-benzenoid aromatic system with 6π-electron 7-carbon-ring structure.[1] Recent synthetic advances by our group have made this unique species much more accessible and understood, allowing us now to start to utilize it for a wide range of applications in organocatalytic chemistry[2-5] 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*

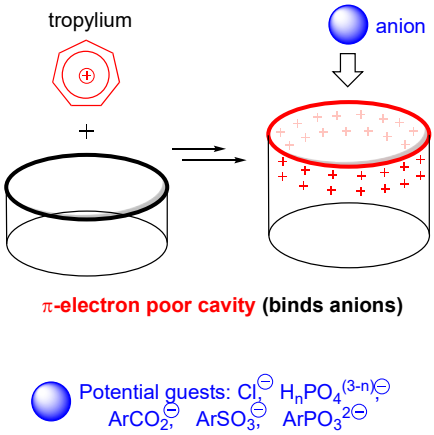
Recently, N-Heterocyclic Olefins (NHOs, see scheme) have emerged as a new class of valuable reaction promoters with interesting action mechanisms. These compounds can be conveniently produced from commercially available precursors in one step. NHOs were originally targeted as a series of active agrochemicals 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.[6] Due to the strong nucleophilicity of the α-carbon, NHOs can act as strong Lewis/Bronsted bases.[7-9] 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.



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CONJOINT A/PROF. GIANCARLO PASCALI

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Radiochemical innovations

Radiopharmaceuticals sciences are a field of research and application at the convergence of chemistry (medicinal, analytical, organic, inorganic), biology, engineering, and pharmacy/medicine. Radiochemical innovations cover a linchpin role in innovating these applications, that ultimately are used to diagnose and treat several diseases.

I have been working in this field since more than 20 years, focusing my research on designing new molecules, devising innovative methods and creating functional machines. More recently, my ongoing interests are in new fluorination strategies, flow/microfluidic reactions, extractive methods for metals and molecular imaging probes. I currently collaborate closely with A/Prof. Luke Hunter at School of Chemistry and other academics on these and other topics.

I am still building up my research space in the UNSW/POWH precinct and currently not able to offer direct laboratory access; however, please make contact if interested to discuss as there might be options to build up collaborative projects with other groups in UNSW.

CONJOINT LECTURER, DR JOHN DOAN

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Radiopharmaceutical Development

Radiopharmaceutical science is a multidisciplinary field encompassing chemistry, physics and biology. It is the science of incorporating a suitable radionuclide into a pharmaceutical or other biologically active molecule in vivo physiological or biochemical processes. The resulting radiopharmaceuticals are used in the diagnostic imaging or therapy of patients with various diseases.

I have an interest in the development of radiopharmaceuticals with potential clinical applications in various fields including oncology and neurology. My role at the Department of Nuclear Medicine and PET, Prince of Wales Hospital is to provide the radiopharmaceutical clinical service for diagnosis of various diseases.

I have recently been appointed as a Conjoint Lecturer and a National Imaging Facility Fellow and I am seeking potential students to work on projects that could enhance the growing field of Radiopharmaceutical Sciences.

DR MARTIN PEEKS

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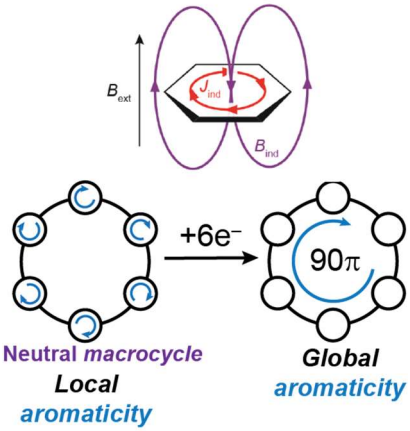
SUPRAMOLECULAR & MATERIALS CHEMISTRY

Our research is concerned with applying the principles of supramolecular and macrocyclic chemistry to make interesting new molecules and assemblies. In doing this we have two real goals: making molecules that have useful properties, and/or that help us learn something new and fundamental about chemistry. The overriding goal of all the projects is to give you the opportunity to **develop a broad set of research skills**: synthesis, computational chemistry, and in-depth analytical or photophysical studies, depending on your interests. There are many options for collaboration with other groups both at UNSW and overseas.

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

(a) Exploring (anti)aromaticity in large macrocyclic molecules

Aromatic molecules have been studied for more than 150 years, but it has only recently become possible to synthesise stable antiaromatic molecules and other unusual pi-conjugated systems. One of our main research areas the properties and applications (e.g. molecular electronics, photovoltaics, magneto-optics) of novel pi-conjugated molecules. We also want to see how we can use these pi-conjugated fragments to prepare huge aromatic rings, larger than ever reported.

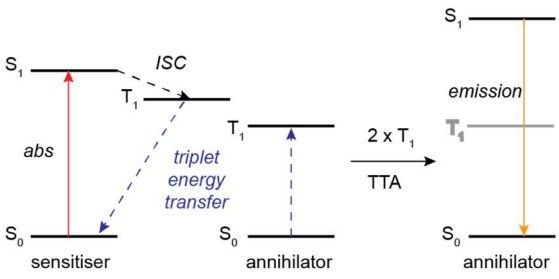


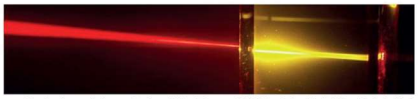
You've probably heard of Hückel's rules, which tell us that molecules with [4*n*+2] pi-electrons are aromatic, and those with [4*n*] are antiaromatic. But this isn't always true. Large macrocycles which comprise lots of aromatic subunits seem not to establish global aromaticity, instead 'preferring' to maintain the local aromaticity of each subunit. Past examples show that oxidation or reduction of the macrocycle is required to promote a global (anti)aromatic ring current,[2] **but we want to see whether we can make large molecules which are (anti)aromatic in their neutral oxidation states**. Large (anti)aromatic molecules are interesting for two reasons: (1) their existence contradicts the received wisdom of textbooks; and (2) the aromatic ring current, which we observe in NMR chemical shifts of aromatic compounds, appears similar to the persistent current in small (~100 nm) metal rings:[3] we need to make bigger (anti)aromatic molecules to see how far the similarities extend, including towards interesting physics in large magnetic fields.

This project spans synthesis, analytical chemistry (NMR, optical spectroscopies), and computational chemistry (DFT analyses of aromaticity).

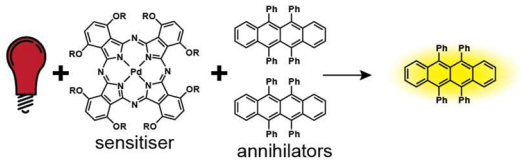
(b) Molecules and assemblies for photon upconversion (with Prof. T. Schmidt)

The process of photon upconversion permits the conversion of low energy (red/near-infrared) light into higher energy light in the visible range. This process is important for two main applications: (1) enabling light-harvesting by photovoltaics across a wider spectral range; (2) powering photochemistry with low energy light, such as for in-vivo applications.





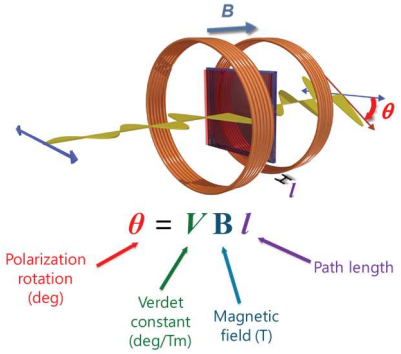
Picture from Schulze, Lips, Schmidt. Proc SPIE, 10.1117/2.1201403.005390



Photon upconversion requires the complex interplay of several different chromophores and their excited states. The relative arrangement of these chromophores in space, as well as their identities, is key for successful upconversion.[4]

The project will involve synthesising a series of organic and inorganic chromophores to systematically explore structure-property relationships. There is an opportunity to use computational chemistry to predict molecular properties, and to measure your new materials in collaboration with the Schmidt group.

(c) Rational design of magneto-optic materials



All transparent materials exhibit an effect called *magneto-optic rotation*, or *Faraday rotation*. This effect rotates the polarization of light, as it passes through a material, in proportion to the strength of an applied magnetic field. This effect is quite important: it's used in photonic devices to control the propagation of light on very fast timescales, and could be used in next-generation magnetic-field sensors. Such materials would be flexible and operative at room temperature: a far cry from the liquid-helium cooled (SQUID) detectors used currently.

Despite the Faraday effect's ubiquity, it's actually quite weak in most materials, except some ferrimagnetic garnet materials – or that was the prevailing wisdom. Recently it's been discovered that a range of organic materials, from polymers through to liquid crystals, exhibit extreme Faraday rotation.[1] So what? Well, the next step from this initial discovery is to learn *how molecular structure controls* the Faraday rotation. With that knowledge, we will be able to logically design new materials with possible applications in healthcare ,self-driving vehicles, and photonics/spintronics.

This project can be attacked in several directions: more synthetic or more supramolecular. You will have the opportunity to make new materials and measure their properties, either directly or in collaboration. We have close links with the Swager group, MIT, on this project. Arrange a chat with Martin to discuss the actual molecules involved!

(d) Other projects

There are lots of other possible projects not listed here. If you're interested in our general area of research, or have your own ideas, please get in touch with Martin to discuss!

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STRUCTURAL CHEMISTRY WITH MASS SPECTROMETRY & ION MOBILITY

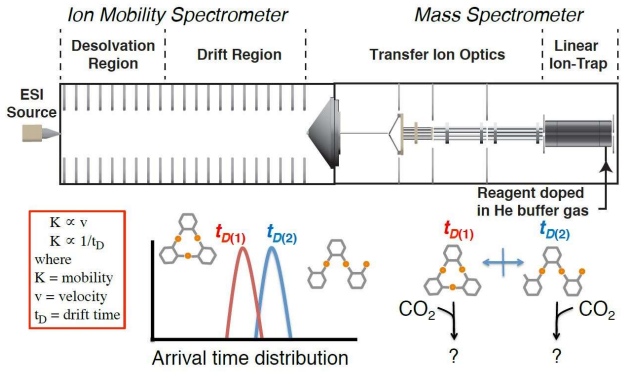
Understanding the intrinsic properties of molecules, molecular building blocks and aggregates is key to realizing the bottom-up design of functional molecules and materials, and catalysts. We explore such molecular units in isolation, for example, via the pristine gas phase environment of specially modified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

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 examining structure. 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 e.g. monitoring the progress of molecular self-assembly reactions. Together ESI-MS and IMS represent two complementary analytical methods of monitoring reaction solutions on a millisecond timescale.

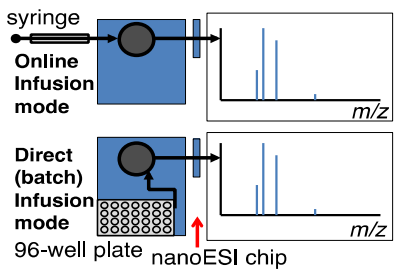
Unique techniques used in the Rijs group include:

- advanced electrospray ionisation mass spectrometry and ion-mobility mass spectrometry (**A**),
- robotic analysis of dynamic combinatorial solutions (**B**), & screening of chemical data sets,
- electronic structure and trajectory methods of computation for structure and function

A IMS-MS enables isomers separation



B High throughput MS with robotics.



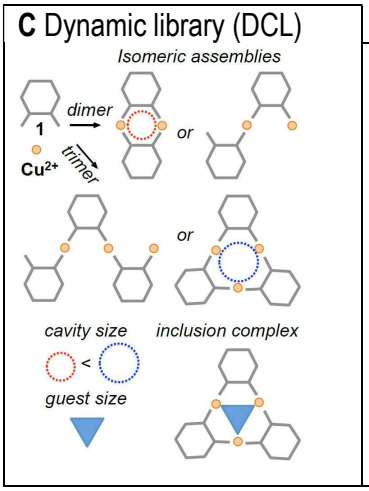
It would be great to work with students on the following projects:

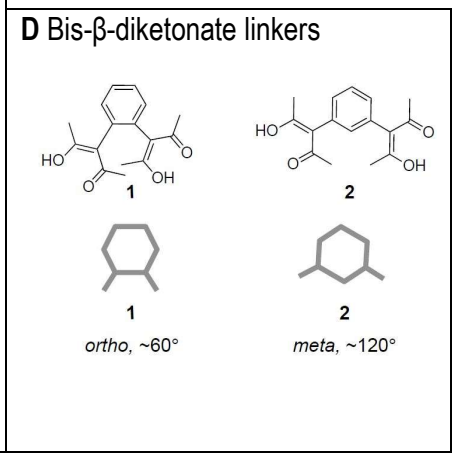
(a) Intercepting critical intermediates from dynamic combinatorial libraries of bis-β-diketonates

Dynamic combinatorial libraries (DCL) are mixtures of self-assembling oligomers in dynamic equilibrium (as illustrated in **C**). Controlling equilibrating species allows one to selectively direct a system. Cu(II) combined with ditopic bis-β-diketonate ligand, 1,2-bis-(3-acetylacetone)benzene (Structure 1, **D**), yields such a mixture of dimeric and trimeric assemblies in solution. These ligands are ideal building blocks for

forming open assemblies capable of encapsulating guest molecules. Depending on the angle of the ligand elbow (e.g., meta-bis-β-diketonates ~120° versus ortho-bis-β-diketonates~60°, **D**), different shaped oligomers are feasible. Small molecules such as amines and solvents, to larger molecules like fullerenes, have been encapsulated by copper bis-β-diketonate assemblies. This makes them ideal targets for gas encapsulation, where specific cavity sizes can be prepared for target gases (e.g. CO_2).

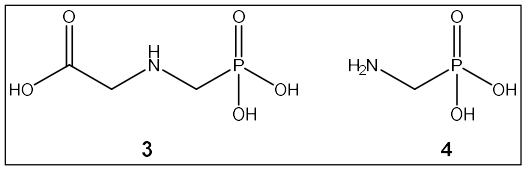
The aim of this project is to develop a methodology for monitoring self-assembly and to direct the synthesis of selective uptake assemblies. Robotically controlled nESI-MS will be used to measure the stoichiometry of evolving molecular assemblies, formed from DCLs.





(b) Mono and dicationic complexes of Glyphosate and Aminomethylphosphonic acid analysed by combinatorial MS

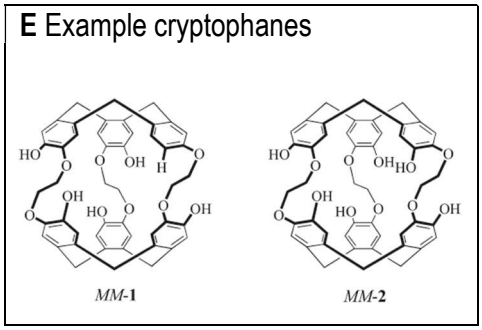
N-(phosphonomethyl)glycine, commonly known as Glyphosate, is a ubiquitous herbicide worldwide. Aminomethylphosphonic acid (AMPA) is the main metabolic product of glyphosate. Metal complexation of this herbicide and its degradation product is an important factor affecting the environmental fate in soil and water. Additionally, AMPA is a weak inhibitor of metalloenzymes e.g. leucine aminopeptidase (a Zn^{2+}-containing metalloenzyme), AMPA's biological activity being linked to its metal complexation properties. A consistent approach to determining the metal binding properties of these two species is the aim of this project.



Glyphosate, **3,** exists in a zwitterionic form with a phosphonate proton delocalized on the amino nitrogen. As a ligand, glyphosate possesses three internal donor sites, (phosphate, carboxylate, amino). AMPA, **4,** is also able to exist in various forms when binding to a metal. A combinatorial approach based on robotics will be used to screen the metal complexes of Glyphosate and AMPA formed in solution.

(c) Encapsulation of ions in solution by cryptophanes probed by ion-mobility MS

Cryptophanes (**E**) are known for their extraordinary complexation properties. They can capture small neutral or charged molecules, such as methane or metal cations. For this reason, they have become functional targets for applications as diverse as gas sensing, environmental remediation, and hosts for MRI contrast reagents.



In this project, ion mobility mass spectrometry will be used to study the complexation and binding affinities of a diverse series of cryptophane complexes, towards explaining the origins of the complexation properties.

Interested students are highly encouraged to discuss their specific research interests directly.

PROF. TIMOTHY SCHMIDT

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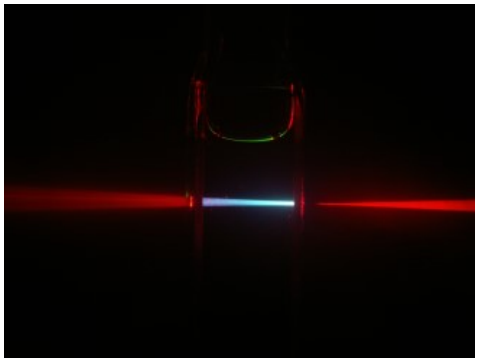
MOLECULAR SPECTROSCOPY AND SOLAR ENERGY

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



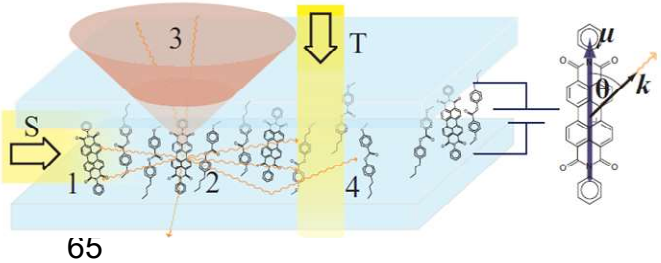
Light from the sun reaches us as a continuous spectrum. But, to generate a photovoltage in a solar cell, we usually neglect that part of the spectrum with photon energies below the band gap. Such a strategy limits the energy conversion efficiency of solar cells to about 33% (UNSW Si cells have reached 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.

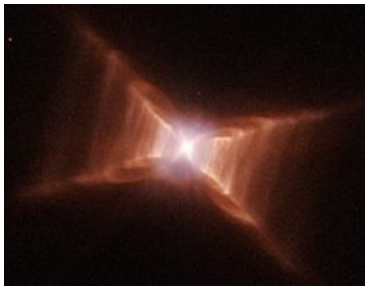


(c) Laser Spectroscopy of Isolated Radicals and Ions (with Prof. Scott Kable)

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.

(d) 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.

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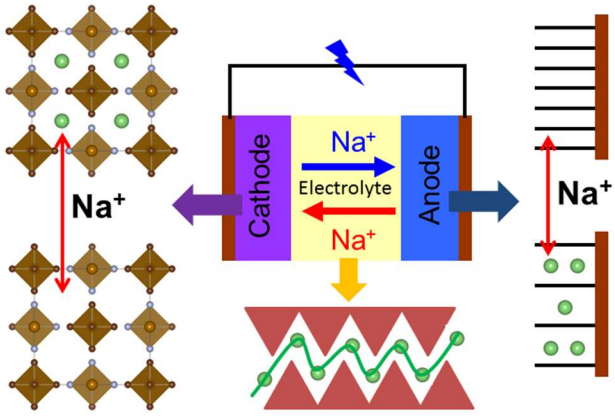
SOLID STATE AND MATERIALS CHEMISTRY

- 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

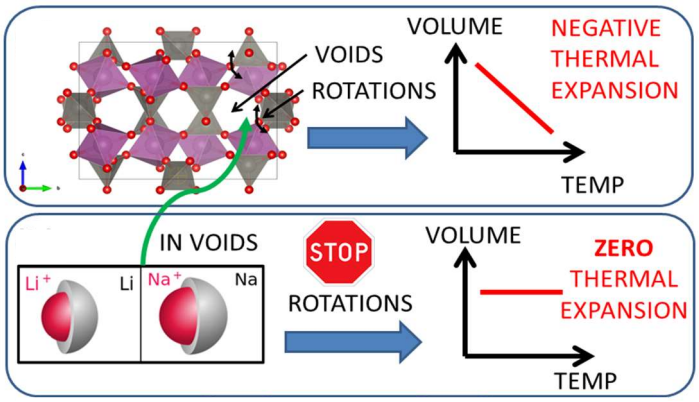
Sodium-ion conducting ceramics or glassy-ceramics are known to be excellent electrolytes at high temperatures (>300°C). This project works towards making materials with sufficient sodium-ion conduction at room temperature.

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 WO_6). 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.

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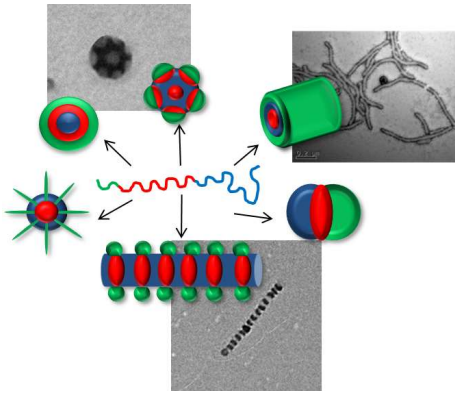
NANOPARTICLES AND TAILORED POLYMERS FOR CANCER TREATMENT

- 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

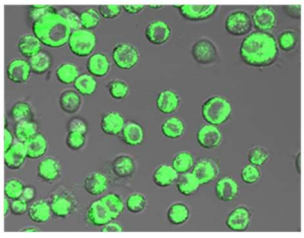


Different nanoparticles prepared from ABC triblock terpolymers

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.

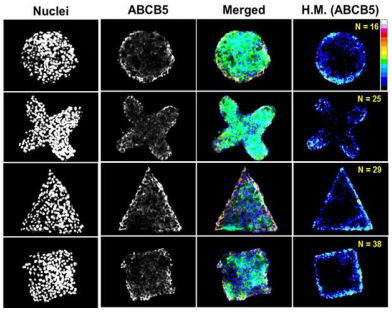
(b) Drug carriers inspired by nature: Nanoparticles with sugar antennae

Carbohydrates are important in a number of biological communication events. 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 using RAFT polymerization has been one of our core activities over the last few years and we would like to use this technology to enhance the delivery of proteins, in particular proteins that assist immunotherapy.



Uptake of nanoparticles with sugar polymers by cancer cells

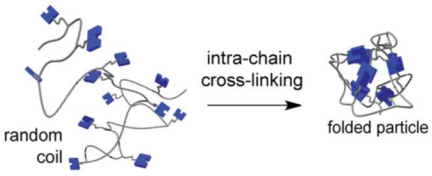
c) Interaction of nanoparticles with cancer stem cells Collaboration with A/Prof Kris Kilian



Nanoparticles are quickly taken up by cancer cells. 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. 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) Making really small polymer nanoparticles

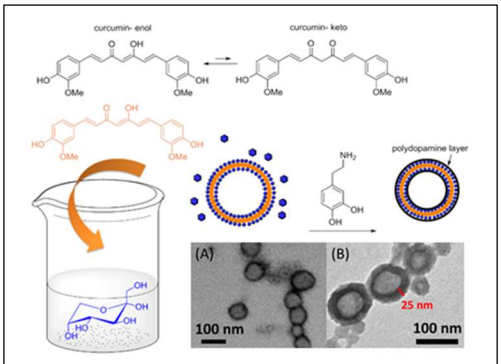
Most nanoparticles described in literature used for drug delivery have sizes above 20 nm. There are however various reasons to make nanoparticles that are even smaller as they seemed to have better circulation time in the blood stream and can diffuse into tumour tissue. To achieve this, we are preparing polymers with attached drugs of various amount and sequence. These polymers are then collapsed into single chain nanoparticles, which are typically below 5 nm in size.



Collapsing of polymer chains into single chain nanoparticles

(e) Nanocapsules

We have recently discovered that mixing of sugar and curcumin can result in vesicle formation. This vesicle is not stable and requires further coating in order to obtain a stable capsule. This capsule can now be used to deliver curcumin to cancer cells, but we can also prepare this capsule with a range of drugs. We would like to explore further the type of drugs that can be loaded, but we are also interested in testing different coating strategies. At the moment the capsule was stabilized by polydopamine, but we would like to explore other strategy such as coating with conducting polymers.



Nanocapsule by mixing of curcumin and sugars, stabilized by a polydopamine shell

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MATERIALS CHEMISTRY AT THE NANOSCALE

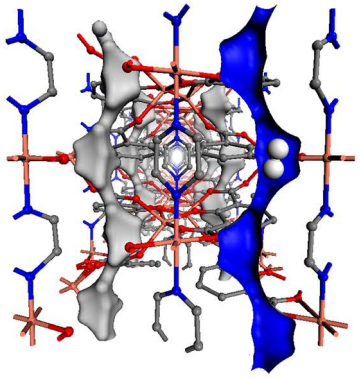
My group focuses on making and understanding new materials that are often focused on some of the major challenges facing us today: energy, water and sustainability. We make use of a range of techniques that include X-ray and neutron scattering in truly multi-disciplinary projects. Key to these studies 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.

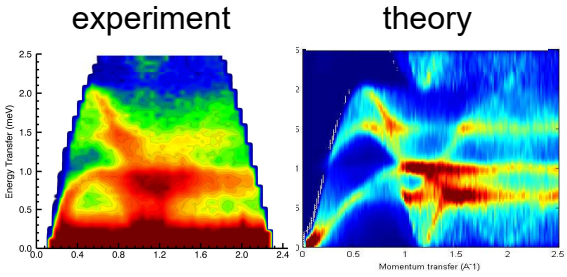
Sorting and storing molecules - how to select for one molecule over another



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 H_2. Highly porous MOFs make excellent host materials for small molecules such as CH_4 or H_2. By tuning their properties MOFs can become efficient storage vessels or effective gas-selective membranes such as the H_2 selecting MOF shown here.

Quantum phenomena in magnetic materials

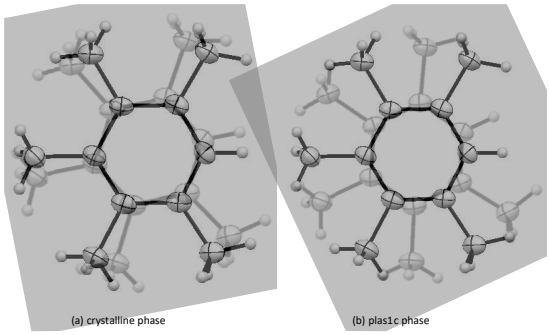
Magnetic materials have revolutionised the way in which we store and use information and have a key role to play in quantum computing; they have also been a navigational aid for centuries and are even pretty useful at securing notes to the fridge door. It is fascinating therefore that we still do not 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.



Spin-wave spectrum of a frustrated magnet using inelastic neutron scattering

(b) Order and disorder in molecular materials

Solid state materials are often though 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.

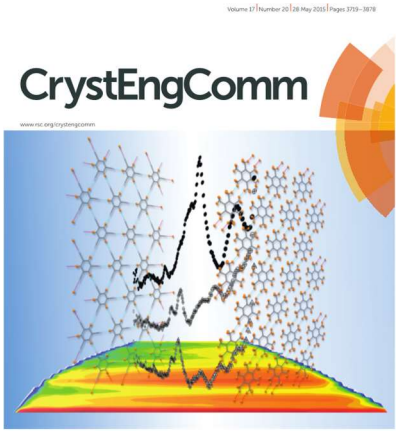


Inter-molecular hydrogen-bonding

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 π-π 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.

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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.

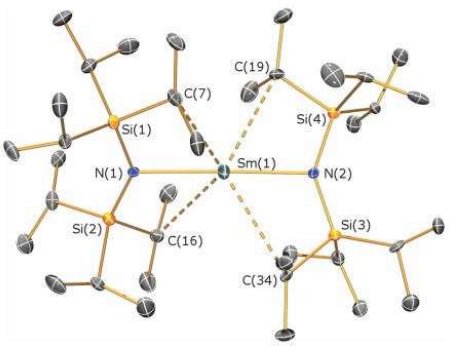
Skills you will learn:

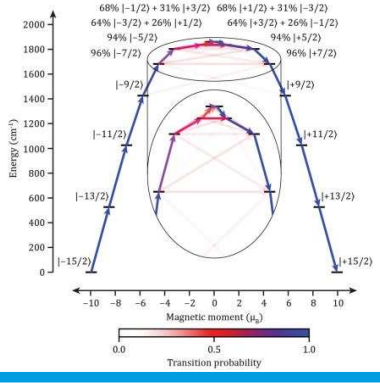
- Manipulation of air- and moisture-sensitive compounds
- Organic and Inorganic synthetic chemistry
- Structure elucidation – NMR spectroscopy (^{1}H, ^{13}C), IR spectroscopy, SQUID magnetometry and XRD (Yeap, we grow crystals)!

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

(a) Sterically hindered low-coordinate lanthanide compounds

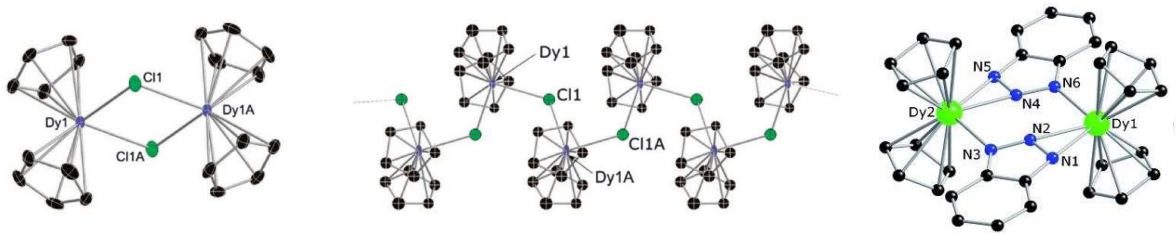
Recent insight into stabilisation of the m_J states of lanthanide containing compounds hints at the potential ability to synthesis compounds that have higher energy barriers to magnetic relaxation than any 3d-block compound. It has been suggested that even subtle changes to the coordination environment 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 unknown[2]… 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…



(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…

1. *Chem. Commun., 2015, 51, 1012.*
2. *Chem. Commun., 2012, 48, 1508.*

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ORIGIN OF LIFE, COMPLEXITY AND NANOMEDICINE

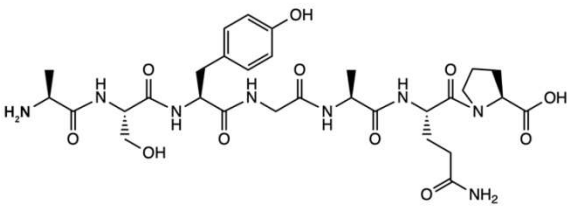
- **Origin of Life and Systems Chemistry,** exploring the role of self-assembly in how life originated and how we can make life-like systems**.**
- **Development** of 3D Cell Culture materials for use in **medical research** and **stem cell therapies**
- **Complexity in Supramolecular Chemistry** investigating the fundamental aspects of host-guest interactions[1]
- **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) Peptide-RNA interactions – solving pressing problems in prebiotic chemistry and medicine *(Collaboration with Dr Albert Fahrenbach & Dr Anna Wang School of Chemistry, Prof. Martin Van Kranendonk, BEES & A/Prof. Archa Fox, University of Western Australia).*

Peptides/proteins and RNA are two of the key building blocks of life. Recently it has become proteins and RNA drive the formation of lava lamp or vinaigrette "droplets"[1] within the cell but biologists are now just uncovering now how important droplet- or gel-like protein-RNA complex are in biology and medicine. At the same time, Origin of Life research[2] has started to turn its attention to a new hypothesis for how complexity could have arisen from a the "pre-biotic soup" of chemicals, particularly peptides and short RNA's.[3] We aim to solve key problems on both fronts by synthesising short RNA and peptides and investigate the structures they form. This would then give clues towards how we could develop medical treatment that modulate these interactions and how we could address one of the most important questions in science, *i.e.*, **how did life originate**. If you join our team to work on these challenges, you would not help us tackling these problems but you will also gain valuable experience in synthesis, self-assembly and the chemistry of RNA and peptide biomolecules such as the peptide shown here:

Did the cell start of as a collection of peptide-RNA "droplets"? And is this how the cell is really organised? (from E. Dolgin, Nature 2018, 555, 300.



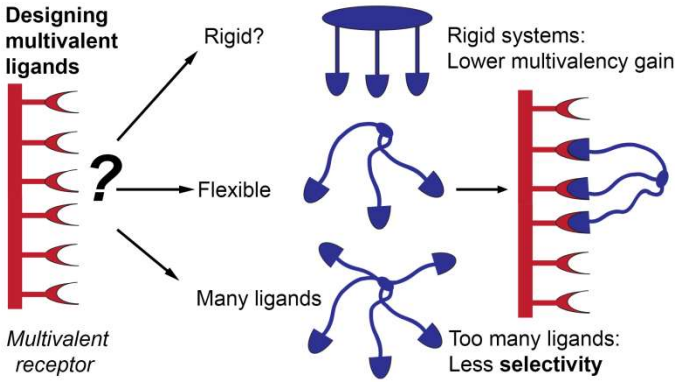
(b) Novel peptides for immunotherapy *(Joint Honours Project with Dr. Angela Finch, SOMS, UNSW).*

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) Multivalency in drug delivery and protein-protein interactions *(collaboration with Dr. Joshua McCarrol and Prof. Maria Kavallaris, Children's Cancer Institute Australia).*

How does the Gecko walk up a wall? How do you stop an influenza virus from binding to and infecting their target cells? The answer to these very different questions centres on the same topic – multivalency! Essentially you need to get a lot of weak interactions to work together, to creating a large effect. The multivalency is also strongly related to another very important topic in biology and supramolecular chemistry - cooperativity.[4]

Despite being known for decades, we still fully understand how the multivalency effect really works on the molecular level and how it can be used to more effectively treat diseases, be it influenza or cancer.[5] But even making a "dimeric" or a "tetrameric" copy of a targeting ligand such as a peptide can have pronounced biological effect – sometimes as much as changing the activity by a 10-1000 fold! Building on recent theoretical advances, we have now a framework (see Figure)[5] to design more effective multivalent system. Projects involving cancer cell targeting[6] and better control over protein-protein interactions, which are important in many diseases ranging from Alzheimer to cancer, are available for anyone that wants to combine synthetic chemistry, supramolecular chemistry and medicinal chemistry in their research training.



1. Elie Dolgin. Cell biology's new phase. *Nature*, **2018**, *555*, 300-302.
2. Pall Thordarson. "Emergence of Life" in *Encyclopedia of Supramolecular Chemistry*: eds: Jerry L. Atwood, Jonathan W. Steed, Marcel Dekker Inc., New York, **2004**, 528-534.
3. Martin Van Kranendonk, David W. Deamer and Tara Djokic, Life Springs, *Scientific American*, August **2017**, 28-35.
4. Larissa K. S. von Krbek, Christoph A. Schalley and Pall Thordarson. Assessing cooperativity in supramolecular systems, *Chemical Society Reviews*, **2017**, *46*, 2622-2637.
5. Kristel C. Tjandra and Pall Thordarson, Multivalency in Drug Delivery – When Is it Too Much of a Good Thing? *Bioconjugate Chemistry*, **2019**, *30*, 503-514.
6. Kristel C. Tjandra, Nigel McCarthy, Lu Yang, Alistair J. Laos, George Sharbeen, Phoebe A. Phillips, Helen Forgham, Sharon M. Sagnella, Renee M. Whan, Maria Kavallaris, Pall Thordarson and Joshua A. McCarroll. Identification of Novel Medulloblastoma Cell-Targeting Peptides for Use in Selective Chemotherapy Drug Delivery. Journal of Medicinal Chemistry, 2019, doi: https://doi.org/10.1021/acs.jmedchem.9b00851 (published 26th July 2019).

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NANOPARTICLE SYNTHESIS & ELECTRON MICROSCOPY

Our group is world leading in the synthesis of the highest performing nanoparticle catalysts and medical imaging agents. Our synthesis expertise allows us to engineer complex nanoparticle catalysts that with atomic level precision. As Director of the Electron Microscope Unit you will use state-of-the-art electron microscopes that are the best in Australia to characterise cutting edge nanoparticles.

Magnetic nanoparticles for cancer detection using Magnetic Particle Imaging

As the first to have a Magnetic Particle Imaging (MPI) instrument in Australia, we are in a unique position to detect early stage tumours and cancerous cells with the most sensitive and precise imaging. The exceptional magnetic properties of iron and iron oxide nanoparticles make these ideal candidates for this state-of-the-art application. These key magnetic properties are dictated by the size, crystallinity and composition of the magnetic nanoparticles.

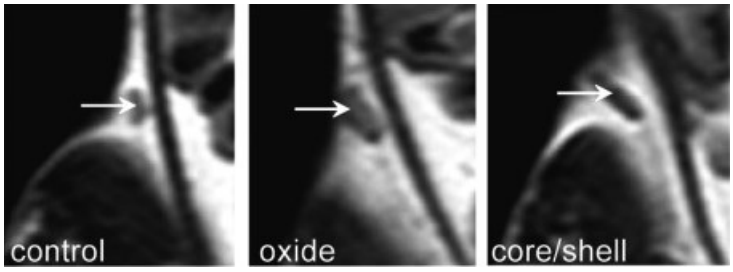

Figure 1: MRI images from iron nanoparticles injected into a mouse to enhance the contrast of a tumour.

Using the leading edge of solution phase synthesis, 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 and collaborate with leading researchers in MPI from Australia. Overall, this work will tune nanoparticle size with precise synthetic control to optimise magnetic properties of iron and iron oxide nanoparticles for MPI.

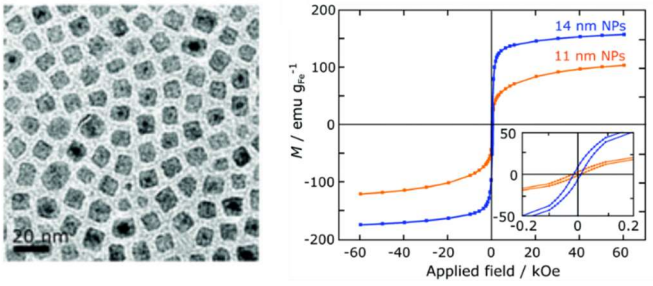

Figure 2: Transmission electron microscopy images of iron nanocubes and their magnetic properties for use in MPI.[1]

1. Gloag, L. *et al.* Zero valent iron core–iron oxide shell nanoparticles as small magnetic particle imaging tracers. *Chem. Commun.* **56**, 3504–3507 (2020).

Controlling nanoparticle structure for active and stable catalysts in renewable energy storage

The oxygen evolution reaction (OER) is crucial for the storage and conversion of H_2 fuel and requires highly active and highly stable catalysts to drive it. Our expertise in nanoparticle synthesis has allowed us to create the most active and stable nanocatalysts for OER reported to date.[1] We achieved this by

synthesizing 3D branched Ru nanoparticles with structural features that both prevent dissolution and improve oxidation catalysis (Figure 1).

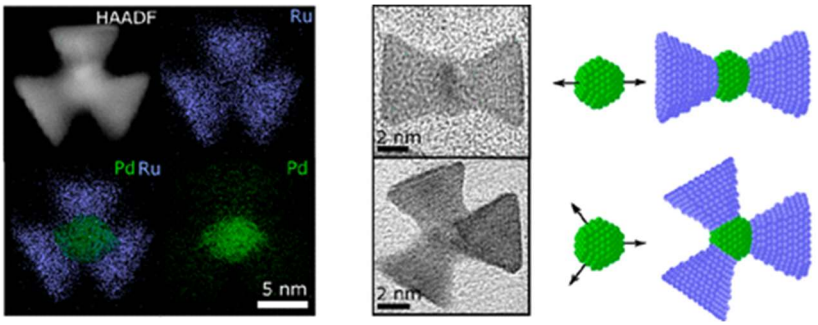

Figure 1: Energy dispersive X-ray spectroscopy elemental mapping of Pd-Ru branched nanoparticles and TEM images of individual nanoparticles. Models show the controlled direction of growth of Ru from Pd seed.

In this project, Ru nanoparticles will be synthesized with low index facets which are critical for achieving stable reaction kinetics that prevent dissolution of Ru and enhance the catalytic activity. This work will combine the development of synthetic methods to control the size, shape and composition of Ru-based nanocatalysts, with advanced characterisation using high-resolution transmission electron microscope and also evaluation of their electrocatalytic performance. This allows for the relationships between nanoparticle structure and catalytic performance to be fundamentally understood and tuned to create leading nanocatalyst materials.

1. Gloag, L. *et al.* A cubic-core hexagonal-branch mechanism to synthesize bi-metallic branched and faceted Pd-Ru nanoparticles for oxygen evolution reaction electrocatalysis. *J. Am. Chem. Soc.* **140**, 12760–12764 (2018).

Synthesising strained Pt on metal nanoparticles for enhanced electrocatalytic activity in hydrogen fuel cells

In order to convert to sustainable energy cells in a hydrogen economy, nanocatalysts need to be high-performing and use minimal amounts of scarce Pt. Strained Pt on the surface of a metal nanoparticle is a promising structure for highly active fuel cell catalysts. Depositing Pt directly onto Ni nanoparticles creates highly strained Pt that maximises the specific and minimises the amount of expensive Pt that is used to provide the highest mass activities reported to date (Figure 1).[1]

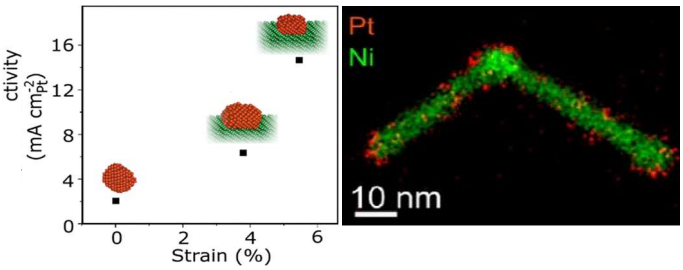

Figure 1: Relationship between strain and HER activity and elemental map of a Pt on Ni nanoparticle.[2]

In this project, nanoparticles will be decorated with small clusters of Pt atoms for use as high performance catalysts. By controlling the position of Pt atoms on different metal nanoparticle structures, both electrocatalytic activity and stability will be optimised to create the most advanced and effective nanoparticle catalysts.

1. Alinezhad, A. *et al.* Direct Growth of Highly Strained Pt Islands on Branched Ni Nanoparticles for Improved Hydrogen Evolution Reaction Activity. *J. Am. Chem. Soc.* **141**, 16202–16207 (2019)

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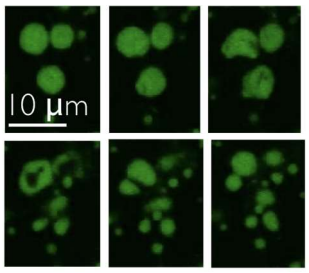
SOFT MATTER BIOPHYSICS AND THE ORIGINS OF LIFE

Some of the most fascinating and poorly understood phenomena in the natural world are, surprisingly, 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 microscopy methods. We use experimental techniques across science and engineering to collect data, and computational tools as much as possible for analysis. There is potential to collaborate with labs in the United States, Japan, and China.

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

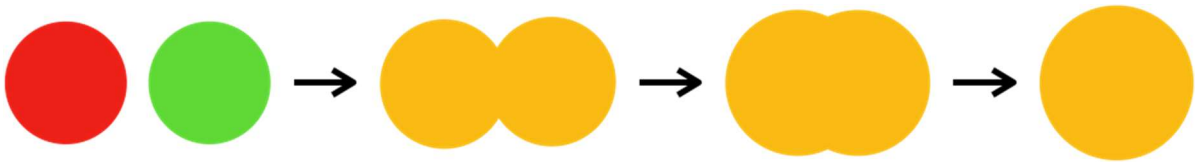
(a) Primitive cell division



Dividing a cell involves a range of shape deformations and cell membrane remodelling. Though these processes are regulated and mediated by proteins in living organisms, proteins in general are unlikely to have been present on early-Earth. How, then, did the earliest cells divide?

This project will examine the potential for inclusions, such as colloidal particles, nanoparticles, and minerals, to alter the local membrane curvature and deform the membrane. Appropriate mineral inclusions will be identified in discussion with geologists at the Australian Centre for Astrobiology.

(b) Primitive membrane fusion



If there are two populations of primitive cells, how often do they fuse and exchange internal material? Such processes would have been critical to jump-start evolution, but stability against fusion is also required to maintain cell integrity.

This project will investigate strategies for inducing moderate levels of primitive cell-cell fusion. The energy barrier for fusion arises from exposing a lipid's hydrophobic regions to water, as well as any electrostatic repulsion that may prevent two membranes from being close enough to fuse. Fusion rates will be monitored by

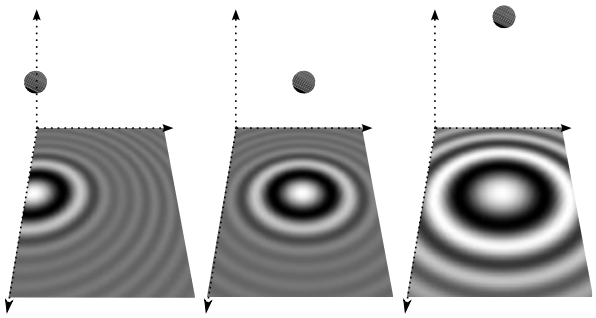
mixing two populations of vesicles labelled with different dyes, and using epifluorescence microscopy to monitor fusion over time.

(c) Permeability and (d) fluidity of a growing membrane

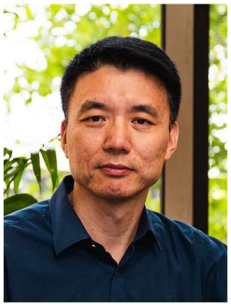
The following two projects are part of a synthetic biology collaboration with labs in the US and Japan. The broader goal is to make a synthetic cell that is capable of synthesising its own membrane, and dividing.

Cells typically have a phospholipid membrane that must grow in order for a cell to propagate. These projects will investigate how the presence of membrane proteins, and the intermediates of lipid synthesis, including lysophosphatidic acids and fatty acids, affect the (c) permeability and (d) fluidity of membranes. Do the precursors make the membrane more or less fluid? How is the lipid packing altered? These results will be applied to designing a synthetic biology system that can continually grow and divide.

(e) Holographic microscopy



There are also several projects related to the development of holographic microscopy as a technique, please email Anna for more details! This exciting technique enables rapid, three-dimensional imaging of cell-sized objects.



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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, CO_2 reduction, gas sensors, cochlear implants, bioimaging, and flexible batteries.

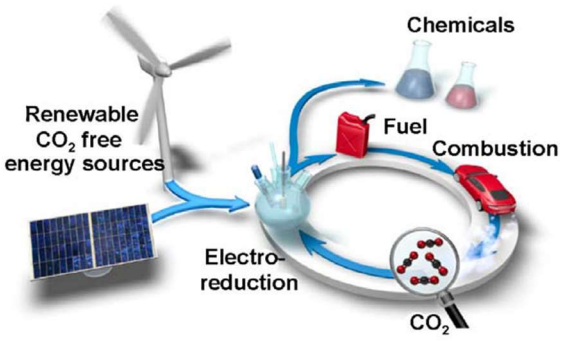
It would be great to work with Honours students on the following projects:

(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 CO_2 to Fuels with Renewable Electricity and Earth Abundant Catalysts

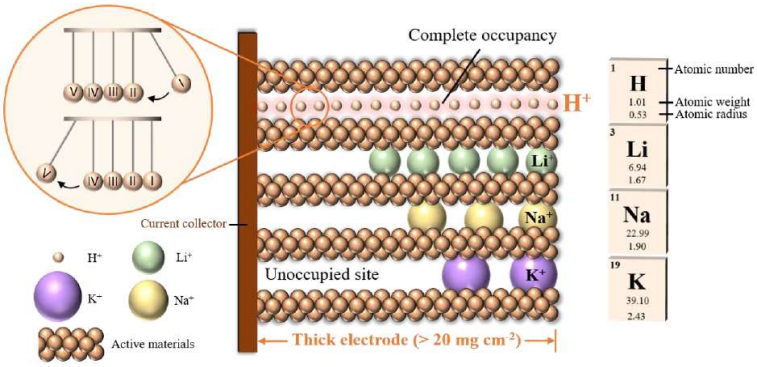
Fossil fuels have historically been the primary feedstock for petroleum based products and industrial chemicals. Apart from the impact that fossil fuels pose on the environment, they are generally mined in remote locations and require massive infrastructure for processing and distribution before they are even refined. One promising solution is to reduce CO_2 itself to petrochemical feedstock, which could cater to the unprecedented consumerism of society and simultaneously reduce the anthropogenic emissions of CO_2 in the atmosphere to restore the natural carbon cycle. To improve the CO_2 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 CO_2 into useful fuels.

(c) Proton Batteries Towards Ultrafast and Sustainable Energy Storage (in collaboration with Dr Neeraj Sharma)

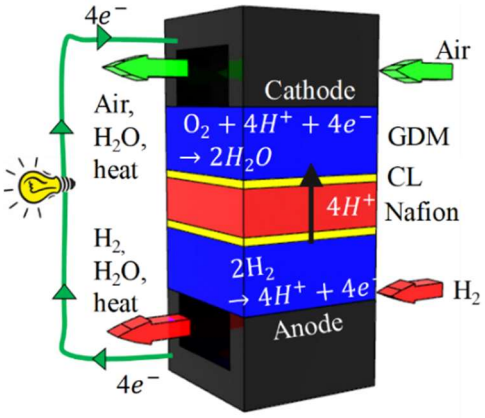
The development of materials that can integrate advantages of high energy density of batteries, and high rate-capability (and long cycle-life) of supercapacitors is of great significant in electrochemical energy storage, yet very challenging to achieve. This is attributed to the intrinsic confliction between the capacity and rate-capability when associating with metal-ion charge carriers (e.g. Li+, Na+, K+, etc.): To exploit higher capacity requires more redox reactions and longer diffusion distances of charge carriers, therefore the corresponding kinetics becomes slow. Fortunately, there recently raises a new possibility of building up an interesting proton (hydronium) chemistry for batteries. Benefitting from small radii and ultrafast transportations in aqueous electrolyte (and even in solid state), proton batteries hold the promise to realize the longing-seek.



This project focuses on designing and synthesizing various materials accessible for proton-species. The student would learn knowledge on material synthesis, standard procedures for evaluating electrode electrochemistry, physical characterizations, and even constructions of real devices. Overall, a comprehensive understanding of energy storage techniques could also be gained.

(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 synthesize 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).

PLuS ALLIANCE

ARIZONA STATE UNIVERSITY PHOENIX | KING'S COLLEGE LONDON LONDON | UNSW AUSTRALIA SYDNEY

HONOURS AT UNSW CANBERRA
School of Physical Environmental and Mathematical Sciences

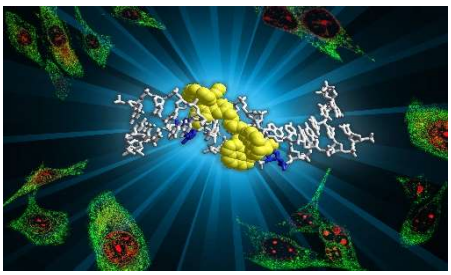
Research into chemistry is also conducted within the School of Physical, Environmental and Mathematical Sciences at the Canberra campus of UNSW. Co-located with the Australian Defence Force Academy, UNSW Canberra maintains a diverse research program and is home to many research students. It is straight-forward 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



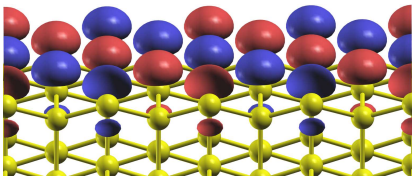
The current focus of our work is in the development of new, and very promising, classes of multinuclear ruthenium complexes as antimicrobial agents. The emergence of drug-resistant populations of microorganisms means there is clearly a need for the development of new antimicrobials — but more importantly, 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

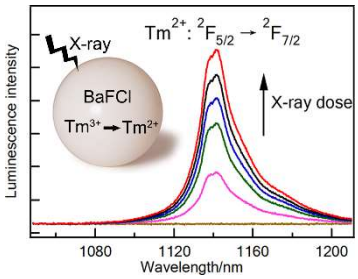


The group's research activities fall broadly under the umbrella of theoretical and computational chemistry, extending into chemical physics. Four main research themes are currently being pursued: Gaussian-based quantum dynamics methods, gas–surface dynamics, dielectric materials, and the structure and 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.

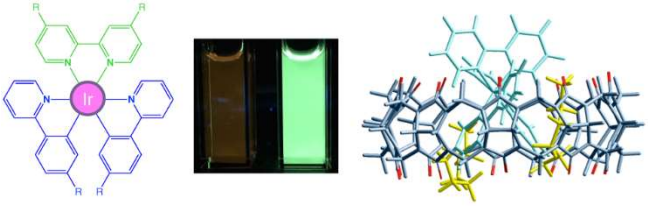
Optical and Laser Spectroscopy of the Solid State — Prof Hans Riesen

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.



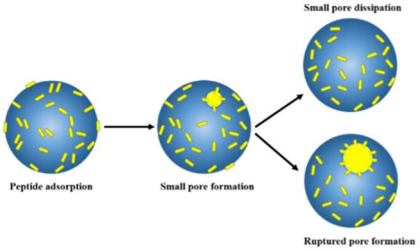
With the advent of the Australian Synchrotron, Hans has also become a user and strong supporter of synchrotron science. In recent years, the group have discovered a novel X-ray storage technology with applications in personal and clinical dosimetry, and medical imaging.

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.