UNSW

School of Chemistry

Honours information booklet

2026

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UNSW School of Chemistry Honours welcome

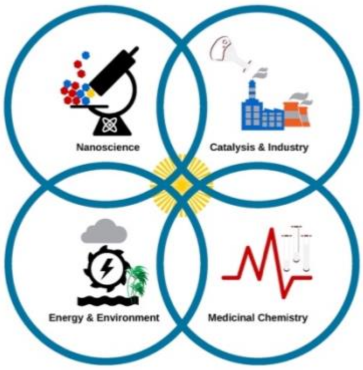
The School of Chemistry at UNSW Sydney is one of the leading centres of chemistry research in Australia.

Composed of over 30 well-respected research teams, we are located in the following buildings on the lower Kensington campus: Dalton (F12), June Griffiths Building (F10), Hilmer Building (E10) and the Science and Engineering Building (SEB).

The School of Chemistry has state of the art research facilities that enable research spanning the breadth of chemistry. The UNSW Mark Wainwright Analytical Centre (MWAC) is co-located adjacent to the School of Chemistry and provides major research facilities that are unsurpassed internationally.

Research in the School of Chemistry can be classified in **four strategic areas:**

- Catalysis & Industry
- Energy & Environment
- Medicinal Chemistry
- Nanoscience



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 has strong links to Australia's professional body for chemists, the Royal Australian Chemical Institute **(RACI)**. Several research team leaders hold senior positions in the RACI, and the NSW state branch is located on campus. The School of Chemistry also has close ties with the International Union of Pure and Applied Chemistry **(IUPAC)** and American Chemical Society **(ACS).**

The School of Chemistry welcomes applicants for Honours from students across the world, acknowledging that Honours is an outstanding introduction to independent research.

We are confident that the wide range of research undertaken in the School of Chemistry provides applicants with a rewarding Honours experience.

Professor Timothy Schmidt (Head of School of Chemistry)

A/Professor Sara Kyne (School of Chemistry Honours Coordinator)

Why do Honours in the School of Chemistry?

Honours in the School of Chemistry offers a unique opportunity to expand your capabilities through independent research and advanced coursework. You will refine your critical thinking, problem-solving, and analytical skills, which are highly valued across many industries.

Benefits of undertaking Honours include:

- Employers in industry and the public value the high-level training received by Honours graduates
- Honours gives you active, hands-on learning experience in a science research environment
- Honours provides you with experience at managing your own project, independence and time management skills.
- Honours may lead to postgraduate study in chemistry
- Honours is an opportunity to become part of a research team in the School of Chemistry, and many consider it a highlight of their university experience

Honours eligibility

For admission to Honours in the School of Chemistry, it is expected that a student will have:

- Bachelor degree specialising in chemistry, medicinal chemistry or related discipline (3-year full-time equivalent)
- WAM average over 65 (credit average)
- Qualifications in other disciplines may also be eligible for admission
- In all cases, enrolment must be approved by the School's Honours Coordinator

Students who have completed pass degree requirements at a university other than UNSW, may be eligible to undertake Honours in the School of Chemistry. In such cases, please contact the Honours Coordinator for clarification.

How to apply for Honours

You can explore the details of our current research supervisors and projects later in this booklet.

You will need to meet with at least **three research supervisors** in the School of Chemistry and receive email confirmation they are willing to supervise your project.

Application Information

For information on the application process, please see:

https://www.unsw.edu.au/science/student-life-resources/honours-how-apply

All applicants (Category A and B)

Under the Chemistry heading use the "apply now" button to submit an "intention to undertake Honours" form.

The form will require you to:

- Upload a copy of your academic transcript
- Nominate your supervisors in order of preference (minimum 3)
- Upload a copy of supervisor confirmation emails

Stand-alone Honours applicants only (Category A)

Also submit a formal application for 4500 Science (Honours):

https://applyonline.unsw.edu.au/login

Please be aware of application closing dates each term. We encourage you to submit your application well in advance of this deadline.

You will be contacted via email to advise the outcome of your Honours application

Honours inquiries

A/Prof. Sara Kyne

Honours Coordinator

Email: chemhonoursadmin@unsw.edu.au

School of Chemistry

Dalton Building (F12)

UNSW Sydney

Overview of Honours

Aims

The overall aim of this course is to provide research training and advanced disciplinary knowledge. Students will develop independent research skills by conducting their research project. The course will develop students' chemistry research skills and competencies, including critical evaluation of data and communication of results.

The **original research project** forms the main component of Honours. Researchers offer projects aligned with their areas of expertise, and you undertake one of these projects under the guidance of an allocated supervisor for the duration of Honours.

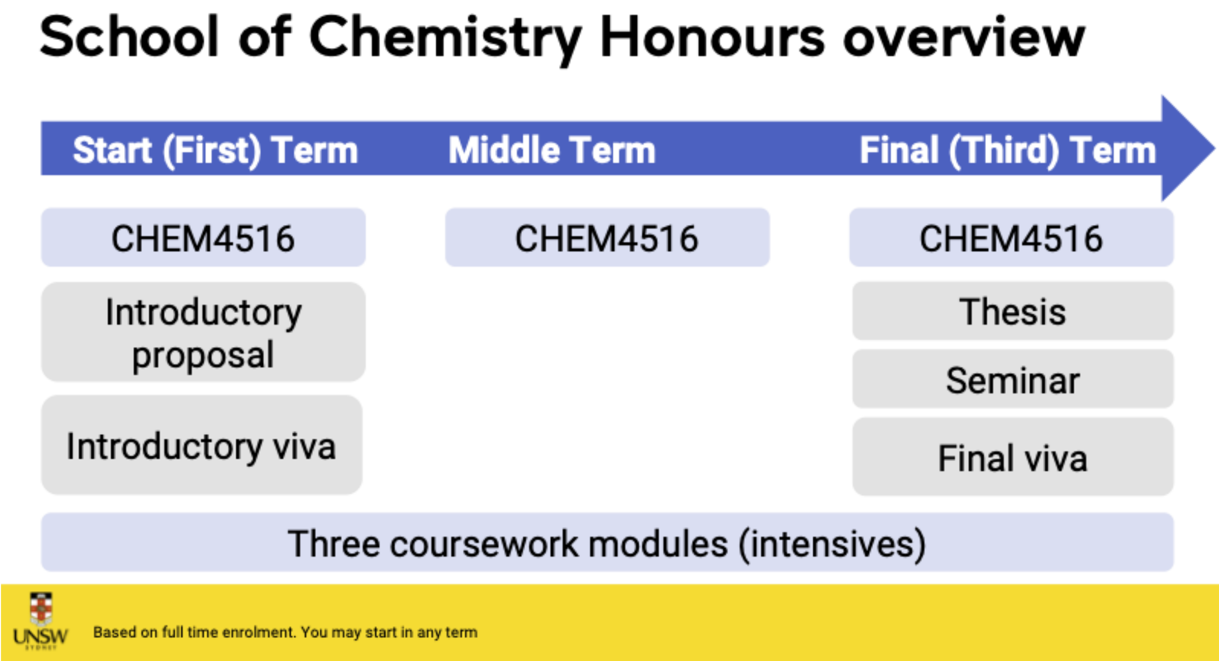
Research skills are developed throughout your research project, including research project planning and execution, proposal writing, data analysis, presentation skills, research ethics and understanding modern occupational health and safety requirements.

Advanced coursework is designed to extend your knowledge and understanding of chemistry. Honours students must undertake three coursework modules offered by the School of Chemistry. These advanced level courses are a combination of theory and skill development.

Research seminars are held throughout the year and are an important means of exposing Honours students to research conducted in the School of Chemistry and at national and international institutions. Attendance is compulsory.

Honours assessments

An overview of the School of Chemistry Honours assessments is shown below.



A summary of each assessment task is given below.

Introductory proposal

The introductory proposal is intended to provide a concise account of your proposed research project. It should demonstrate clarity of thought, describe why the research topic is of interest and the current knowledge base and status in the field. It should describe a research plan for how you intend to tackle the identified problem and the expected outcomes. References (in-text citations) should be used throughout, and a full reference list provided.

You will be provided with written feedback from the examination panel.

Introductory viva

The introductory viva will be similar to a short interview where you give an introductory presentation of your research project (using slides or aids such as a whiteboard if you choose), followed by questions from the examination panel.

The introductory viva will take a maximum of 20 minutes.

Students will be introduced to their examination panel during the session.

You will be provided with written/verbal feedback from the examination panel and your supervisor(s).

Thesis

You will complete a written thesis, submitted at the end of Week 8 in your final term of research.

The thesis should provide a concise and clear account of your research, written in a scientific style suitable for a general chemistry audience. It should demonstrate clarity of thought and insight into the project.

The thesis should contain an introduction to the background of the project and its objectives. It should detail the research undertaken including the methodology/experimental details, critically analysis of the results and provide a discussion to contextualise the findings. Conclusions should be drawn from the research and highlight future project directions. References (in-text citations) should be used throughout, and a full reference list provided.

You will be provided with written feedback from the examination panel.

Seminar

The seminar is a graded formal presentation of the research project, given to the School of Chemistry. It is held after submission of the Honours thesis.

The seminar comprises a maximum **15 minute** presentation followed by **five minutes** of questions from a public audience.

You will be provided with written/verbal feedback from the examination panel and your supervisor(s).

Final viva

The final viva will be similar to a short interview where you give a brief overview of the project, followed by questions from the examination panel.

The final viva will probe your understanding of the project in detail.

The final viva will take a maximum of 20 minutes.

You will be provided with written/verbal feedback from the examination panel and your supervisor(s).

Coursework

Coursework is offered in intensive mode across all terms.

Coursework will feature a combination of lectures, workshops, tutorials and self-directed study to emphasise the concepts being taught. Each concept would be examined following its completion to consolidate learning. Students are advised at least two weeks before any assessment is given/due.

Coursework will be assessed through a variety of methods including assignments and examinations.

You will be provided with written/verbal feedback from the instructors delivering the coursework within 10 business days.

Honours class boundaries

- 85 and above (H1)
- 75–84 (H2:1)
- 65–74 (H2:2)
- 50–64 (H3)

UNSW

School of Chemistry

Honours supervisors

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A/PROF. GRAHAM BALL

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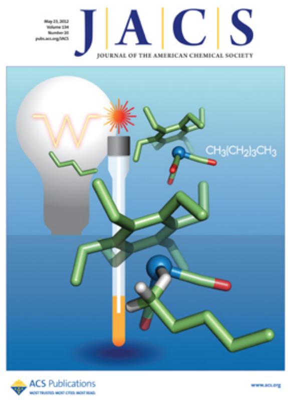
NMR SPECTROSCOPY AND COMPUTATIONAL CHEMISTRY: APPLICATIONS TO ORGANOMETALLIC AND BIOLOGICAL CHEMISTRY

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

(a) Short-lived metal complexes and reactive intermediates

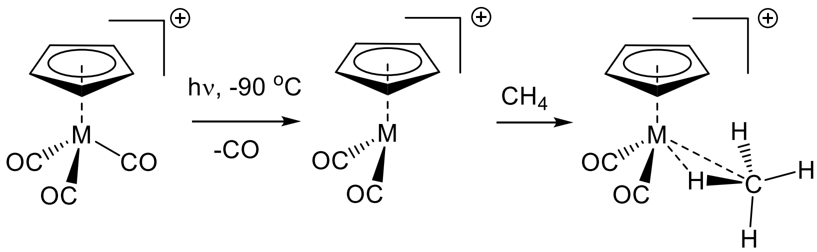


We use photochemistry in combination with *in situ* NMR at low temperatures to study molecules that have fleeting existence at room temperature. With this strategy, we have observed several types of alkane complex,[1-3] including the *JACS* cover opposite,[1a] and even complexes where xenon acts as a 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).

(i) *Alkanes: Binding and Beyond (in collaboration with Prof. Les Field and Dr James Watson)*

Chemists around the globe have been working on ways of converting relatively unreactive alkanes found in petroleum into useful compounds using a process known as C-H activation. Alkane complexes are key short-lived intermediates in the activation process.

Currently, this ARC funded project is aimed at answering questions such as: Can we make more stable alkane complexes? Can we do chemistry with the alkanes when they are bound? When bound to a cationic metal centre, the alkane should be activated towards conversion into molecules with functional groups, which would be revolutionary new chemistry! We have recently achieved exciting results observing group 8 complexes (M = Fe, Ru, Os) of the most important alkane, methane.[2,3] There is plenty of scope for students to make new methane or other alkane complexes, with the long-term goal of converting the bound alkane into useful products.



(ii) Computational design of new exotic molecules: 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 above were designed computationally prior to observation.[2,3] Can we design, then observe more stable alkane complexes or complexes with ligands that bind even more weakly e.g. Xe and Kr even?

Projects in these areas 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 three components can be blended to suit the interests of students tackling the project.

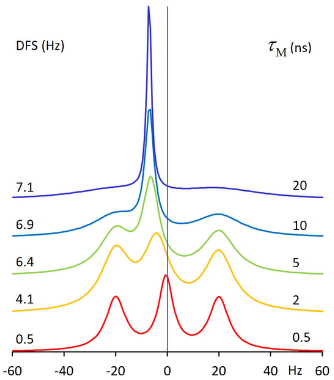
1 (a) Young, R.D.; Lawes, D.J.; Hill, A.F.; Ball, G.E. *J. Am. Chem. Soc.*, **2012**, *134*, 8294. (b) Yau, H.M; McKay, A.I; Hesse, H.; Xu, R.; He, M.; Holt, C.E.; Ball, G.E. *J. Am. Chem. Soc.* **2016**, *138*, 281. (c) Young, R.D.; Hill, A.F.; Hillier, W.; Ball, G.E. *J. Am. Chem. Soc.*, **2011**, *133*, 13806.

2 Watson, J.D.; Field, L. D.; Ball, G.E. *Nature Chem*, **2022**, *14,* 801–804. doi:10.1038/s41557-022-00929-w.

3 Watson, J.D.; Field, L. D.; Ball, G.E. *J. Am. Chem. Soc.*, **2022**, 144, 17622-17629. doi:10.1021/jacs.2c07124.

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

(b) New methods for measuring X-H bond lengths using NMR spectroscopy

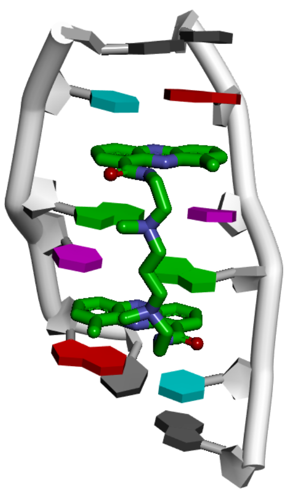


Unlike organic chemistry, where bonds involving hydrogen atoms have predictable lengths, inorganic chemistry is awash with compounds where X-H bond lengths vary significantly, especially when these bonds bind to metals. Hydrogens are very difficult to locate using X-ray crystallography, so new methods for measuring X-H bond lengths are needed!

We are using various NMR techniques, including the little-known dynamic frequency shift (left) to measure stretched H-H bond lengths[5] and we are developing relaxation methods to measure bond lengths in systems containing stretched C-H, B-H and N-H bonds.

5. Gilbert-Wilson, R.; Das, B.; Mizdrak, D.; Field, L.D.; Ball, G.E. *Inorg. Chem*. **2020**, *59*, 15570.

(c) Anti-cancer drug-DNA interactions (in collaboration with A/Prof Larry Wakelin, A/prof Luke Hunter 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 mono and 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.[6,7]

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.

6. Serobian, A.; Pracey, C. P.; Thomas, D. S.; Denny, W. A.; Ball, G. E.; Wakelin, L. P. G. *J. Mol. Recognit.* **2020**, *33*, e2843.

7. Rowell, K.N.; Thomas, D.S.; Ball, G.E.; Wakelin, L.P.G. *Biopolymers*. **2021**, *112*, e23409.

PROF. 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

(collaborations with Prof. Tim Schmidt, Prof. Dean Astumian, Maine, Prof. Ayusman Sen, Penn State)

We are designing and synthesising small molecules capable of performing controlled motion or selective guest binding tasks. A 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: *J. Am. Chem. Soc.* **2020**, *142*, 20014–20020; *J. Phys. Chem. Lett.* **2021**, *12*, 1236–1243.

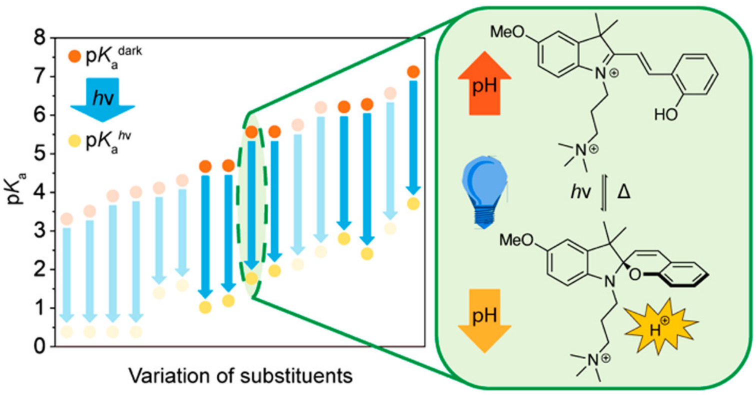
(b) Molecular photoswitches

(collaboration with Dr Felix Rizzuto; Prof. Palli Thordarson, Prof. Joakim Andreasson, Gothenburg; Prof. Bart Jan Ravoo, Munster; Prof. Dave Adams, Glasgow, …)

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, switching ON/OFF catalytic activities, binding interactions, or changing material properties such as in hydrogels.

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



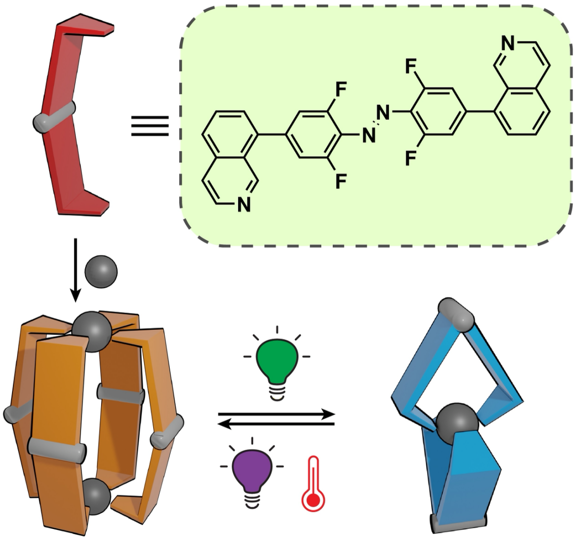
Relevant publications*:*

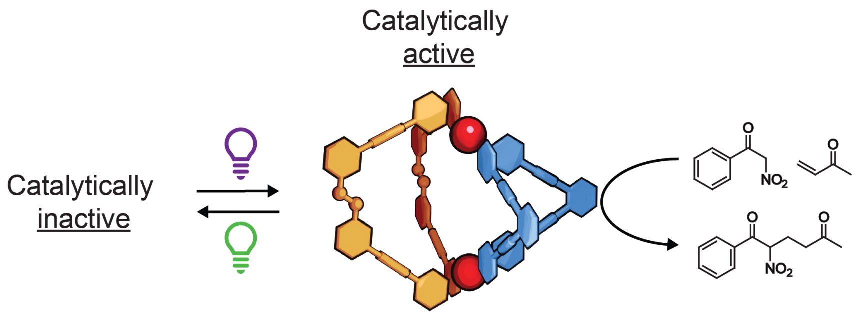
J. Am. Chem. Soc. **2023**, *145*, 2088–2092; *J. Am. Chem. Soc.* **2021**, *143*, 20758–20768; *Chem. Commun*. **2022**, *58*, 5610-5613; *ChemPhotoChem*, **2020**, *4*, 407-412; *Chem.- Eur. J.* **2020**, *26*, 1103–1110.

(d) Self-assembly of functional structures

(collaboration with Prof. Paul Lusby, Edinburgh; Prof. David Amabilino, Barcelona)

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 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: *J. Am. Chem. Soc.* **2024**, *146*, 21196–21202; *Angew. Chem. Int. Ed.*, **2022**, *e202205701; Chem. Eur. J.* **2022**, *28*, e2021044*; Chem.- Eur. J.* **2020**, *26*, 1103–1110. *Chem.- Eur. J.* **2019**, *25*, 5708-5718.

(e) …other projects tailored to your interests!

Our other interests cover areas ranging from NMR to microfluidics to polymer chemistry!

DR. JEFFREY BLACK

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CHEMISTRY EDUCATION AND ToF-SIMS

The Chemical Education group at UNSW is focused on improving the learning experience and outcomes of students studying chemistry in a scholarly manner, contributing to the global chemistry and science education communities.

While our primary focus is on tertiary chemistry students, it may be applicable to other subjects, especially other sciences as well as secondary education or education in general. As such we welcome potential students with diverse backgrounds in science and/or education.

My personal interest is in the use of technology to assist with learning and assessment including as preparation for other activities, complementing learning activities, standalone learning activities, and improving assessment and feedback practices with the use of technology. Additionally, I have a passion for lab work and am eager to explore the development of new laboratory experiments to enhance student learning while providing an authentic experience.

Projects may involve intervention design and evaluation; engaging with chemistry students through learning activities such as labs, workshops and tutorials; interviews and questionnaires/surveys of students and staff; artifact/data collection; as well as both qualitative and quantitative analysis of data.

Digital Assessment (in collaboration with Dr Siobhán Wills)

With technology becoming more widely used in all aspects of life, the use of pen and paper based assessment appears very much out of place. However the shift to digital assessment brings along its own opportunities and challenges. Some important questions are how students perceive digital assessment and if any groups are advantaged or disadvantaged by this shift.

Projects in this area may include new digital assessment techniques and tools; tools to prepare students for digital assessment, or evaluation of student interactions, performance and perceptions of digital assessment.

Technologically assisted assessment (in collaboration with Dr Siobhán Wills)

Even with assessment remaining as pen and paper, there is opportunity for assessment to be enhanced with technology, such as measures to prevent collusion, increasing efficiency of marking, providing students with better feedback, or the use of technology to assist students in completing the assessment.

Projects in this area may include designing new tools or evaluating existing tools to determine their effectiveness of preventing and detecting collusion, the efficiency of the assessment preparation and marking process, the usefulness of feedback provided to students, and any student or staff perceptions on the process.

Virtual labs for increased preparation and performance

Coming into a chemistry lab for the first time can be a daunting experience, with lots of equipment and glassware that may not have been seen before, in a new space, with new techniques needing to be performed, along with potentially hazardous chemicals. This places a significant cognitive load on students and may make their performance in the lab suffer. By providing virtual lab experiences students can be safely introduced to the lab environment in advance of their laboratory class, making the space a more familiar environment when it comes time for their lab class. It can also allow them to interact with the lab, equipment and glassware to practice techniques in a safe environment to focus more on the experiment and understanding the chemical principles during their laboratory classes.

Projects in this area may include the development of virtual lab tours or virtual lab experiments; and the evaluation of student interaction with these tools and what impact it has had on the learning experience and performance of the student.

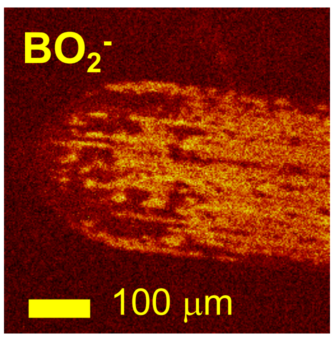
Other Chemistry Education projects of your choosing.

I am happy to entertain any other ideas you may have for chemical education projects. If you have any ideas or questions, feel free to speak to to see what is possible. Collaborations between academics researching Chemical Education at UNSW (or more broadly) for new projects are also possible.

ToF-SIMS for analysis of tribological surfaces. (collaborators include Drs Jonathan Palmer, Chris Marjo, A/Prof Jason Harper and Prof. Chris Tierney, UNSW; Prof. Larry Scott, Boston College; Prof.'s Sergei Glavatskih and Mark Rutland, KTH, Stockholm)

My other passion is research in sustainable materials and processes for a sustainable future with a current focus on developing an understanding of how lubricants are transformed during use with the aim of producing better, and longer lasting lubricants.

Time of Flight – Secondary Ion Mass Spectrometry (ToF-SIMS) allows probing the 3D distribution of chemical species in a solid surface. This allows developing an understanding of the breakdown and tribofilm formation pathways of lubricants, including how different species can influence further breakdown and formation; and how this process evolves over time.



ToF-SIMS analysis showing the breakdown products of an orthorborate ionic liquid in a wear scar after a lubrication test.

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.

PROF. ALEX DONALD

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FUNDAMENTAL & APPLIED MASS SPECTROMETRY

Mass spectrometry is a pivotal technology driving advancements in both established and emerging scientific fields. Under the leadership of Prof. Alex Donald, our team is developing and implementing cutting-edge experimental methodologies in mass spectrometry with a particular focus on challenges in chemistry and biochemistry. We are seeking students who are eager to acquire a highly valuable skill set in mass spectrometry and related disciplines, and who are motivated to contribute to exciting research that bridges fundamental science and real-world applications. Expertise in mass spectrometry is highly sought after in industry, government, and academic labs, spanning a wide range of fields in science.

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

(a) Advanced Biomarker Discovery Using Mass Spectrometry and Artificial Intelligence

Cancer remains one of the most challenging health problems we face today. While some cancers can be treated effectively if caught early, the prognosis for late-stage cancers is often grim. For example, pancreatic cancer is notoriously difficult to detect in the early stages, which contributes to its low survival rate of just 10%, largely because diagnosis usually occurs at a late stage. Wouldn't it be great if we could catch cancer much earlier, before its spread, and when treatment is far more likely to be successful?

Mass spectrometry is a powerful technology that can detect incredibly trace amounts of molecules in biological samples, making it an ideal tool for early cancer detection. Unlike imaging methods, which can only detect cancer once it's large enough to be seen, mass spectrometry has the potential to identify cancer long before it becomes visible, by spotting tiny changes in the levels of certain molecules—known as biomarkers—in the blood or tissue.

But there's a problem: traditional methods of biomarker discovery often consider each biomarker in isolation, looking for individual molecules that signal the presence of cancer. This approach misses out on the bigger picture. The reality is that many biomarkers are linked, and it's their ratios and complex relationships that might give us the clearest indication of early-stage cancer.

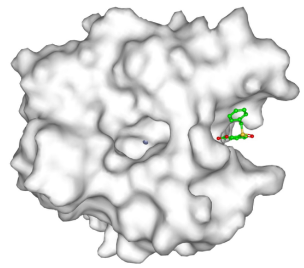
Last year we reported a groundbreaking computational framework called CRANK-MS, which uses machine learning to analyze large, complex datasets from mass spectrometry. CRANK-MS doesn't just look at individual biomarkers; it uncovers intricate relationships between them. By analyzing how the levels of different biomarkers are coupled together, we can potentially detect cancer far earlier than current methods allow.

Neural network framework for predicting diseases using large mass spectrometry-based 'omics data.

This approach is poised to significantly advance early-stage cancer diagnostics. By applying this method to challenging datasets, we aim to significantly improve the accuracy of early detection, giving patients a much better chance at successful treatment and survival.

(b) Multiplexed Screening of Molecular Libraries Using Native Mass Spectrometry

Small molecules that bind to proteins are the foundation of many modern medical treatments, from cancer therapies to cardiovascular drugs. These interactions are key to modulating protein activity, making small molecules essential in the development of new drugs. However, the traditional process of discovering these molecules is slow and labor-intensive. Typically, researchers must screen one molecule at a time, which requires extensive purification, curation, and storage of large libraries of compounds. This not only slows down the drug discovery process but also limits the number of molecules that can be realistically screened.



Methods for rapidly screening pooled mixtures of small molecules for binding to druggable targets are needed to accelerate the drug discovery process.

The solution to this challenge lies in multiplexed screening using native mass spectrometry, a groundbreaking approach that allows us to screen vast, unpurified combinatorial libraries of small molecules simultaneously. By employing our brand-new Ultra-High Mass Range (UHMR) Orbitrap mass spectrometer, we can potentially screen hundreds of thousands to millions of molecules at once. This technique eliminates the need for DNA tags or other cumbersome identification methods, streamlining the screening process and dramatically increasing throughput.

Through this project, students will learn valuable synthetic chemistry skills, enabling them to create these large combinatorial libraries. Additionally, they will gain expertise in native mass spectrometry, a cutting-edge technique that is rapidly becoming essential in drug discovery. The focus of this research is on drug targets involved in cancer, making this work not only technically challenging but also critically important for developing new cancer treatments.

(c) Decoding Carbonic Anhydrase Proteoforms: Impact on Function and Interactions

Proteoforms are distinct molecular forms of a protein, arising from genetic variations, alternative splicing, or post-translational modifications. They are crucial for understanding biological complexity and disease but have been relatively understudied due to challenges in their characterization. The methods for identifying and studying proteoforms, mainly advanced mass spectrometry, are still in their infancy.

Our research focuses on carbonic anhydrases, enzymes vital in many physiological processes, especially in red blood cells, where they regulate acid-base balance. These enzymes are important drug targets for conditions like cancer and Alzheimer's. Recently, we discovered that small chemical modifications to carbonic anhydrases, catalyzed by other enzymes, can drastically alter their catalytic activity and interactions with clinically approved drugs. This suggests that traditional drug testing, which usually considers only the primary form of a protein, might miss crucial therapeutic potentials or risks linked to different proteoforms.

This project addresses this gap. You will purify carbonic anhydrase from red blood cells and use advanced intact protein mass spectrometry, along with other cutting-edge methods, to identify and characterize their proteoforms and their interactions with drugs. This work is crucial for developing drugs specifically designed to target disease-relevant proteoforms, potentially leading to more effective and personalized treatments. Moreover, this approach may change the paradigm for how target-based drugs are discovered and optimized by focusing on more relevant and realistic protein forms.

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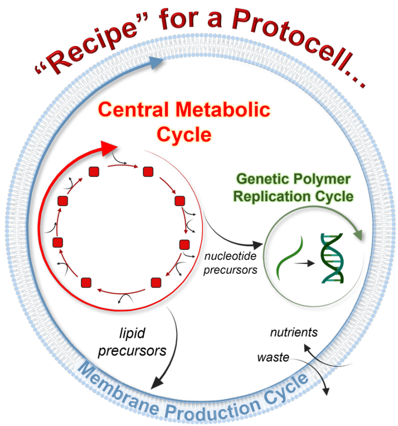
Director of the Australian Centre for Astrobiology

ORIGINS OF LIFE ORGANIC CHEMISTRY



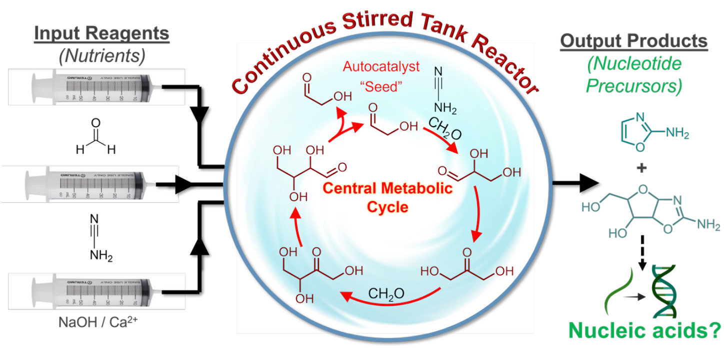
Ever thought about how life got started? Are you interested in astrobiology? Then consider doing your honours with my group!

My group seeks to develop experimental and theoretical models for understanding how "life-like" behaviours can emerge from simple chemical systems. *We are particularly interested in developing and understanding autocatalytic reaction networks that can be exploited for the construction of a simple protocell "from scratch".*

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

(a) Optimising Autocatalytic Syntheses for RNA Precursors

(Co-supervisor: Associate Professor Giancarlo Pascali, School of Chemistry)



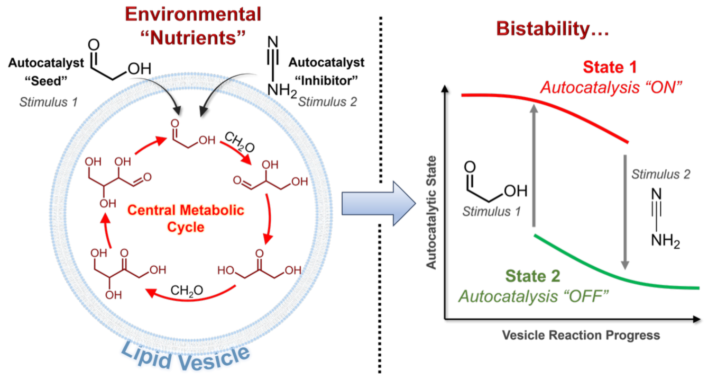
Autocatalysis is an essential feature of life. The cell utilizes a variety of different autocatalytic reactions to carry out metabolism. Autocatalysis affords not only dynamic "life-like" behaviours, but also provides a mechanism for reproduction at the molecular level. In fact, you might consider the entire process of cellular reproduction a complex suite of coupled autocatalytic reactions.

While the cell is a master of autocatalysis, we still don't understand very well how to utilize autocatalysis in synthetic contexts. The aim of this project is to optimise an autocatalytic reaction network, known as the formose reaction, for production of RNA precursors using a continuous stirred tank reactor (CSTR).

Unlike your typical organic reaction, which takes place inside of a round-bottom flask and so must eventually come to equilibrium, a CSTR is an open system, continually supplied with fresh reagents pumped into the reactor, while products are likewise continually removed at the same rate. To a first approximation, a CSTR allows one to carryout synthesis more like the cell does, which constantly takes in nutrients from the environment while expelling waste. More than just fundamental science, we expect this type of autocatalysis carried out within a CSTR to lead to novel methodologies for production of commercially important synthetic compounds.

(b) Autocatalytic Reaction Networks in Vesicles for Emergent "Life-Like" Behaviours

(Co-supervisor: Dr Anna Wang, School of Chemistry)

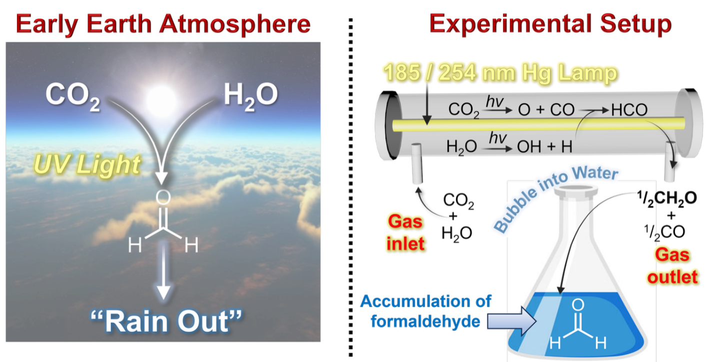


The cell is a master of autocatalysis, but we still don't understand the fundamentals of autocatalytic react-ions when carried out in cell-sized compartments. This project aims to demonstrate "life-like" behaviours made possible when autocatalytic reactions are carried out within the confines of a protocell – a model for a simple cell based on lipid vesicles.

One of the cell's most fundamental life-like features is bistability. Bistability refers to the fact that many metabolic processes can be switched "on" or "off" (hence are bistable) depending on a variety of factors such as nutrient supplies in the environment. Under the right circumstances, autocatalytic reactions afford mechanisms for achieving bistability, being able to turn themselves on and off in response to exposure to appropriate chemical stimuli. In this project, we aim to show that the autocatalytic formose reaction when carried out inside of a lipid vesicle can be turned on and off by different chemical stimuli, molecules which can be considered as environmental "nutrients". Showing this sort of bistability in a protocell vesicle will reveal how even relatively simple molecular systems can lead to life-like emergent behaviours that allow a protocell to respond to its environment "intelligently".

(c) Autocatalysis Starting from Atmospheric Chemistry

(Co-supervisor: Dr Chris Hansen, School of Chemistry)



The autocatalytic formose reaction depends on the constant supply of formaldehyde (CH_2O), but how could formaldehyde have been made available on early Earth during the age of prebiotic chemistry around 4 billion years ago? This project aims to demonstrate that formaldehyde could have been produced atmospherically by the photochemical reaction of CO_2 and H_2O, which then "rained out" onto the early Earth's surface.

Given the lack of an ozone layer, the flux of UV-light penetrating the early troposphere especially in the 200–350 nm region is suspected to have been much greater in comparison to today. Moreover, the partial pressure of CO_2 is thought to have been as high as ~100 bar. In this project, we aim to model experimentally the atmospheric synthesis of formaldehyde using a custom-built UV reactor that takes into account these early Earth atmospheric conditions. We expect to see the accumulation of formaldehyde by passing the gaseous reaction mixture through an aqueous solution, mimicking the early Earth's surface. Demonstrating accumulation of formaldehyde will support the idea the autocatalytic formose reaction could have occurred on early Earth some 4 billion years ago.

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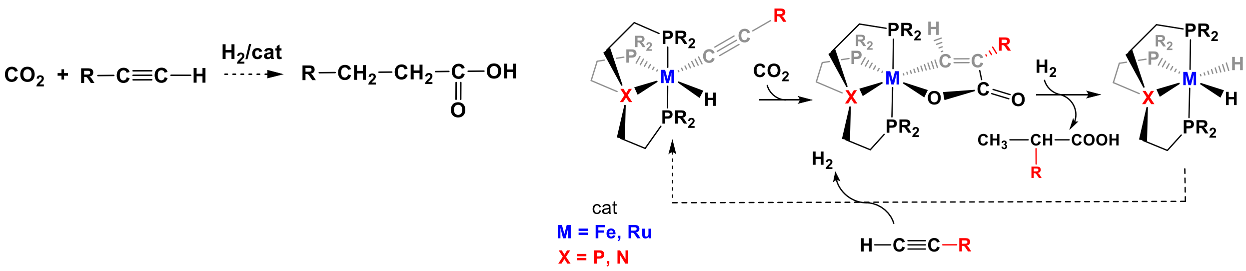
SYNTHETIC ORGANOMETALLIC CHEMISTRY

- Research in the Field group is centred around synthetic organometallic chemistry:
  - Development of organometallic catalysts that activate small molecules (such as N_2, CO_2, CH_4 *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:
  - Organic & organometallic synthesis; 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, electrochemistry and X-Ray diffraction.

(a) New catalysts for converting CO_2 to useful organic compounds (with Dr James Watson)

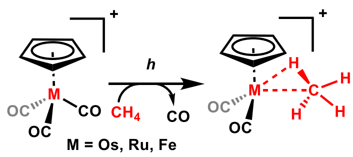
Efficient and high yielding conversion of CO_2 into value-added products remains one of the greatest challenges for chemistry to tackle climate change. We are working on the design of a range of organometallic compounds which react with CO_2 and add it to organic substrates to produce useful organic compounds such as carboxylic acids, esters and carbonates. This turns CO_2 from an environmentally dangerous waste product into a more valuable chemical feedstock.

Projects involve the synthesis of new Fe and Ru complexes that react with CO_2 to give new complexes that can be cleaved to release a CO_2-containing organic compound, and free the metal complex to react again. The cycle uses CO_2 as a 1-carbon building block to make useful organic compounds.

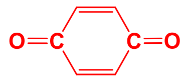


(b) Alkane binding to metals (with Associate Professor Graham Ball and Dr James Watson)

Alkanes are amongst the most inert and unreactive compounds. By careful design, we have been able to make metal complexes that will even bind to the C-H bonds in alkanes. While the metal-alkane complexes are typically short-lived and stable only at low temperatures, we are now making complexes that are much more stable (stable near room temperature) and where we can promote reaction of the bound alkane to make new organic compounds. We have been mostly working with cationic metal complexes of Re and Os and we are extending the study to complexes of Ru, Fe and Mn and also group-9 metals (Rh and Ir). We characterise the compounds using advanced ^1H and multinuclear NMR spectroscopy.

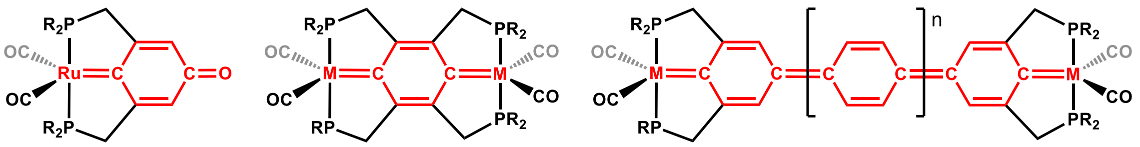


(c) Metal-to-metal communication via cross-conjugated frameworks (with Dr Martin Peeks)



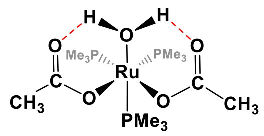
p-quinone

Quinones are a class of organic compounds which have a rich redox-chemistry, and which are heavily used as oxidizing agents both by chemists and in biology. Metallaquinones are analogues of quinones where one or both oxygen atoms are replaced by metals. This project involves making new bi-metallic or polymetallic quinonoid compounds and examining the metal-to-metal electronic communication through the cross-conjugated organic framework. The bi-metallic and polymetallic quinonoid compounds are a new class of organometallic compounds. The results from this project will provide insight into the nature of the metal-to-metal communication and could underpin the design of the next generation of molecular conductors, molecular semiconductors and molecular switches.



metallaquinone dimetallaquinone polymetallaquinone

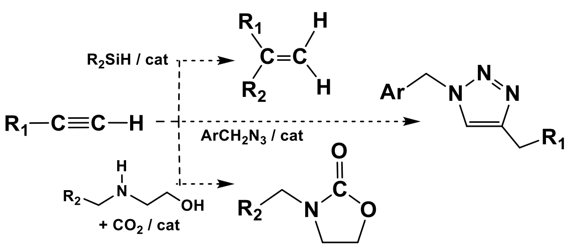
(d) New Ru water complexes for catalytic hydrogenation (with Dr Sara Kyne)

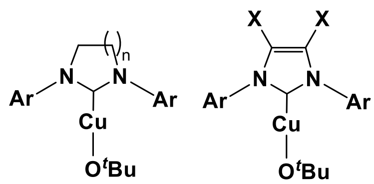


We have recently discovered a series of ruthenium carboxylate complexes $[Ru(PMe_3)_3(RCOO)_2(H_2O)]$ which strongly bind water. The carbonyls of the carboxylate ligands form a perfect pocket to bind a molecule of water with strong hydrogen bonds between the carbonyl oxygens and the water protons. These are remarkably stable metal complexes, and they are active as catalysts for the homogeneous hydrogenation of simple alkenes. The initial project is to improve and optimize the catalysts by *(i)* modifying the molecular structure (varying the carboxylates to drive stronger or weaker hydrogen bonding; varying the phosphine supporting ligands to influence the steric environment around the metal and electronic properties of the Ru centre); *(ii)* working out the mechanism for hydrogenation and this will drive optimization of the catalyst; and *(iii)* by tuning the reduction conditions (quantifying the catalyst efficiency, optimizing catalyst loading, temperature, pressure *etc*). We will also examine the potential reduction of other functional groups (esters, carboxylic acids, amides, nitriles *etc*).

(e) Copper(I) NHC complexes for C-C bond formation (with Dr Samantha Furfari)

Terminal alkynes can be functionalised with silanes, aminoalcohols and organic azides using Cu(I) catalysts containing *N*-heterocyclic carbene ligands (NHCs). This project will synthesise a series of copper(I) complexes, modifying the NHC ligand structure to optimise the catalytic conversion of alkynes to substituted alkenes, oxazolidones and triazoles.





Selected publications:

1. Binding Methane to a Metal Center. J. D. Watson, L. D. Field and G. E. Ball; *Nature Chem,* **2022**, *vol. 14, no. 7,* pp. 801–804; doi:10.1038/s41557-022-00929-w.

2. $[Fp(CH_4)]^+$, $[\eta^5\text{-}CpRu(CO)_2(CH_4)]^+$ and $[\eta^5\text{-}CpOs(CO)_2(CH_4)]^+$: A complete set of Group 8 metal-methane complexes. J. D. Watson, L. D. Field and G. E. Ball. *Journal of the American Chemical Society,* **2022**, *vol. 38, no. 144*, pp. 17622-17629; doi: 10.1021/jacs.2c07124.

3. Dinuclear Acetylide-bridged Ruthenium(II) Complexes with Non-aromatic Spacers. S. Naik, S. Ø. Scottwell, H. L. Li, C. F. Leong, D. M. D'Alessandro, L. D. Field, *Dalton Transactions*, **2020**, *49*, 2687–2695; doi: 10.1039/C9DT04856A.

4. Fe(0)-Mediated Reductive Disproportionation of CO_2. P. M. Jurd, H. L. Li, M. Bhadbhade, L. D. Field, *Organometallics*, **2020,** *39,* 2011−2018; doi.org/10.1021/acs.organomet.0c00175.

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CHEMICAL EDUCATION RESEARCH & ORGANOMETALLIC SYNTHESIS

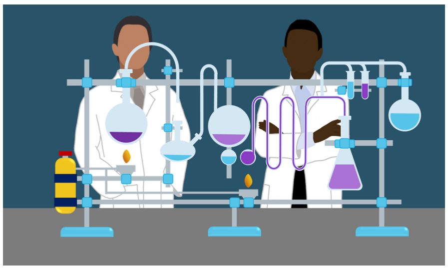
Research in the **SynthED** group is centred around two areas: **chemical education** and **synthetic organometallic research**. The **chemical education** projects are focussed on the **practical curriculum** and **inclusive education**. Research into the **practical curriculum** includes creating and assessing, new experiments and materials that will enhance the learning experience, improve safety and efficiency, and support diverse educational needs. **Inclusive education projects** aim to create a more equitable and inclusive learning environment by addressing systemic barriers and developing strategies to ensure that all students can succeed and thrive in the field of chemistry by using a research-led approached.

The **synthetic organometallic** projects are focussed on the development of metal complexes for small molecule activation and catalytic processes. These projects are investigating **new approaches** for C-C and C-X bonds formation with a high degree of chemo-, regio- and stereoselectivity as well as the development of **electron reservoir ligands** for small molecule activation.

Chemical Education Projects

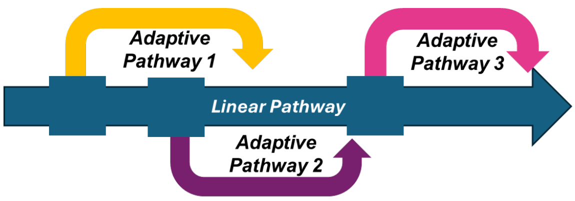
In the chemical education projects, you will gain experience in **(i)** Design and implementation of support teaching for the undergraduate laboratories. **(ii)** Analysing quantitative and qualitative data through different avenues such as questionnaires, focus groups and interviews. **(iii)** Communication skills through the dissemination of these results to a wider teaching audience **(iv)** Project management **(v)** Awareness of equality, diversity and inclusion issues

(a) **Experimental Development for Practical Chemistry** (in collaboration with Dr Peter Rayner & Dr David Pugh, University of York, UK)



We are continuing efforts to incorporate contemporary experimental methods across all year levels of the chemistry undergraduate. We will evaluate new experiments by assessing skill acquisition through pre- and post-tests, performance metrics, and retention measures, while also collecting student feedback on engagement and challenges via surveys and interviews. This approach provides a comprehensive view of both teaching effectiveness and student experience.

(b) **Development of Online Resources for Undergraduate Teaching Labs** (in collaboration with Dr Ron Haines & Dr Laura McKemmish)



A growing area of interest is the use of Adaptive Tutorials (ATs), which are a way to allow students to learn at a pace that suits them and provide tailored support from afar. We are interested in developing the use of ATs in the teaching labs to enable students to be better prepared experimental chemistry and assess their effectiveness using both quantitative measures (time spent in the adaptive pathways compared to the linear pathway) and qualitative feedback (questionnaires and interviews).

(c) Integrating sustainability and green chemistry into the chemistry curriculum (in collaboration with Dr Sara Kyne and Dr Martin Peeks, UNSW)

We aim to future-focus the curriculum, to prepare undergraduate students to tackle global challenges confronting modern society. To achieve this, we are designing and implementing context-based learning activities that link fundamental chemistry concepts with modern society using a systems thinking approach. Our goal is for students to use chemistry to change their individual actions and develop multidisciplinary solutions to sustainability's "wicked problems". In addition to measures such as academic performance, student satisfaction and engagement, these activities will be evaluated based on impact on students' motivation and changes in perceptions towards sustainability as influenced by the enhanced curriculum.

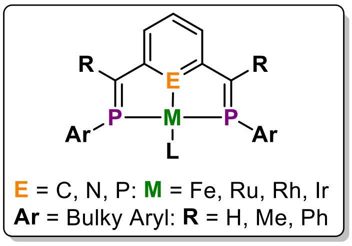
(d) Decolonisation and Diversification of the Chemistry Curriculum (in collaboration with Dr Sara Kyne, UNSW)

Decolonising chemical education involves reshaping curricula to include diverse perspectives and contributions, fostering an inclusive academic environment. To evaluate this project, we will measure the impact of curriculum changes on students' sense of belonging by comparing baseline data on perceptions of inclusivity with follow-up data. We will also assess changes in student engagement, performance, and feedback to determine the effectiveness of the interventions in promoting equity and a sense of belonging.

Synthetic Organometallics Lab Projects

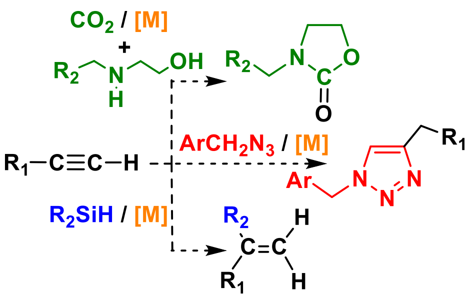
In these synthetic organometallic projects, you will gain experience in: **(i)** Organic and organometallic synthesis, which will include air and moisture sensitive compounds. **(ii)** Characterisation of ligands and organometallic complexes using NMR spectroscopy (heteronuclear & 2D), IR spectroscopy, electrochemistry and X-Ray diffraction **(iii)** Optimisation and evaluation of catalytic reactions.

(a) Development of Electron Reservoir Ligands for Small Molecule Activation and Catalysis (in collaboration with Prof. Les Field)



This project aims to address the reliance of expensive reducing agents of metal mediated nitrogen fixation processes by combining the successful elements of metal-based fixation and electron reservoir ligands in a single molecular unit. This would be a remarkable development in the field that could potentially lead to mild catalytic systems that would greatly reduce the environmental cost that the current industrial processes impart.

(b) Catalysts for C-C and C-X Coupling Reactions (in collaboration with Prof. Les Field)



The focus of this projects is the functionalisation of unsaturated hydrocarbons. Terminal alkynes can be functionalised with silanes, aminoalcohols and organic azides using Cu(I) catalysts containing *N*-heterocyclic carbene ligands (NHCs). This project will synthesise a series of copper(I) complexes, modifying the NHC ligand structure to optimise the catalytic conversion of alkynes to substituted alkenes, oxazolidones and triazoles.

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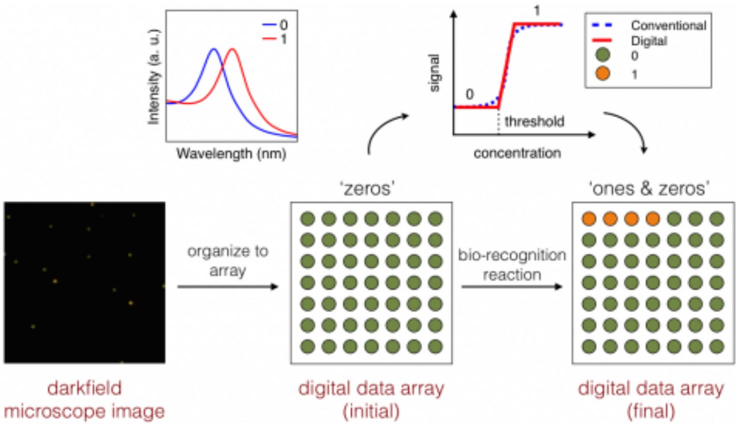
Australian Centre for NanoMedicine

SMART MATERIALS AND SURFACES

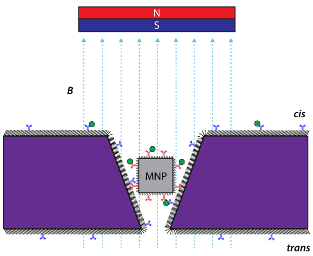
Our research group specializes in using self assembled monolayer or other surface modification technique to provide surfaces with unique functionality. The surfaces are the base upon which we build functional devices from nanscale component including polymer, protein, nanoparticles, and porous material.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

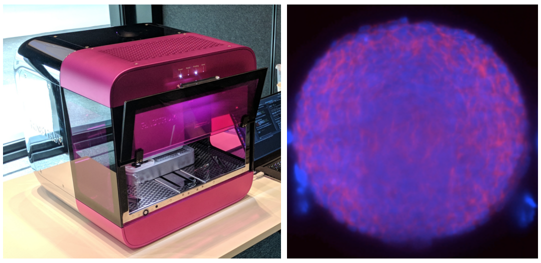
Detection of Single Biomolecules using Magnetic Nanoparticles and Nanopore Sensors



Specific antigen-antibody binding

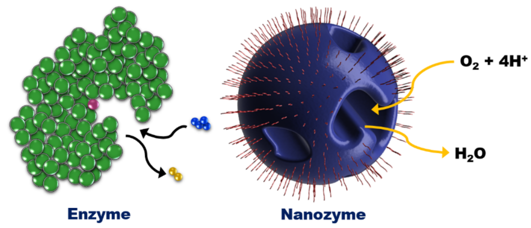
A typical biosensors detects many molecules to give the concentration of species. Nanopores, which are commonly proposed for DNA sequencing, can detect single molecules and give concentration of species by counting many single molecules. This avoids the need for calibration however, detection limits 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 project will involves developing the next generation of this exciting single molecule sensor.

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



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

The synthesis of electrocatalysts for 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 compounds absorb light. I am concerned about the true environmental fate of anthropogenic fluorinated compounds and interested in the molecular environment of interstellar space. Use fundamental physical chemistry/chemical physics to address problems in atmospheric science and astrochemistry!

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

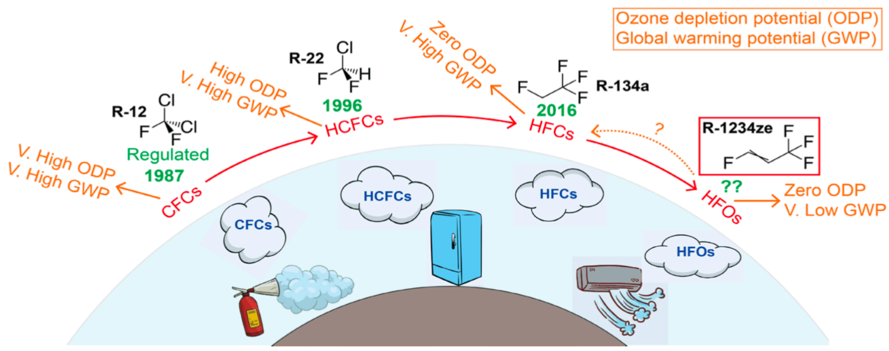
Hydrofluorocarbons (HFCs) are the replacements to the chlorofluorocarbons (CFCs) and hydrochlorofluorocarbons (HCFCs). They have no ozone depletion potential yet still present an enormous risk to the environment as powerful global warming agents. These HFCs have a high infrared activity and long atmospheric lifetimes (decades to centuries) leading to global warming potentials (GWPs) up to 10s of 1000s of times worse than CO_2. An important aim of my research is to improve the underpinning science that is incorporated into atmospheric chemistry models so that humankind can understand the environmental risk of new compounds before they are emitted in large quantities.

(a) UV Photochemistry of Fluorocarbonyls (with Prof. Scott Kable)

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.

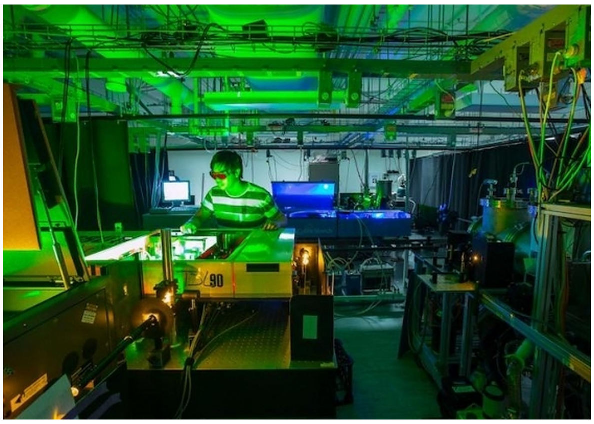
Current HFC replacements incorporate reactive chemical subunits (*e.g.* double bonds) that reduce their atmospheric lifetime to weeks. However, the most likely fluorine-containing end-products have a higher risk to the atmosphere than the compounds being replaced. This project aims to identify these 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 ~12 000 times worse than CO_2.

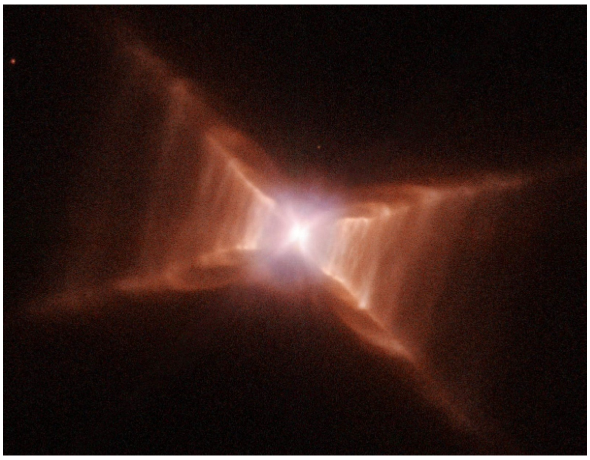


What you will do: Velocity-mapped ion imaging, Fourier-transform infrared (FT-IR) spectroscopy, chirped pulse Fourier-transform microwave spectroscopy, computational chemistry.

(b) Interstellar Molecules (with Prof. Timothy Schmidt)



The *Molecular Photonics Laboratories* house 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.



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* (DIBs), 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 and radicals (which are the leading candidates for carrying the DIBs), and (hopefully) solve this long-standing problem.

What you will do: Laser spectroscopy, electric discharges, vacuum techniques, quantum chemistry

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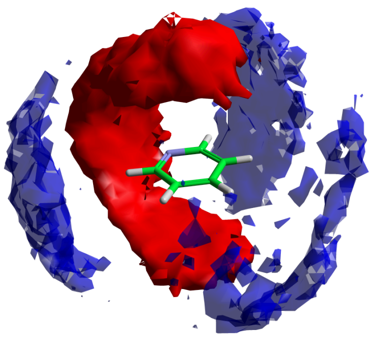
MECHANISTIC AND PHYSICAL ORGANIC CHEMISTRY

Our research is focussed on understanding how organic processes happen and what affects reaction outcomes. Particularly, this work encompasses examining how structural features in both the reagents themselves and the solvent used 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 projects are currently underway in catalysis, reaction kinetics, synthesis and molecular dynamics simulations.

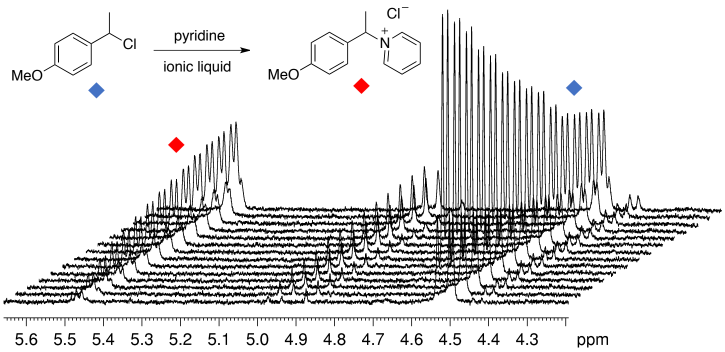
a) Ionic liquid effects on organic reactions: understanding solvation, designing better solvents and getting the reaction outcomes you want.[1] (collaborators include Dr Ron Haines & Prof. Stuart Prescott, UNSW; Prof. Anna Croft, University of Loughborough, Dr Christof Jäger, AstraZeneca, Sweden; Prof. Bill Price, WSU; Prof. Tam Greaves, RMIT)

Ionic liquids are salts that melt below 100°C. They have the potential to replace volatile organic solvents but outcomes of reactions in ionic liquids are often different to those in traditional molecular solvents. The aim of this project is to understand the nature of solvation in these systems – the interactions between a solute and the ions of the ionic liquid – through analysis of reaction outcomes, measurements of solution properties (such as diffusion) and molecular dynamics simulations. The result would be to extend the understanding of these solvent effects we have developed and to use this knowledge to control reaction outcome.



A molecular dynamics simulation showing the organisation of the **cation** and **anion** of an ionic liquid around **pyridine**.

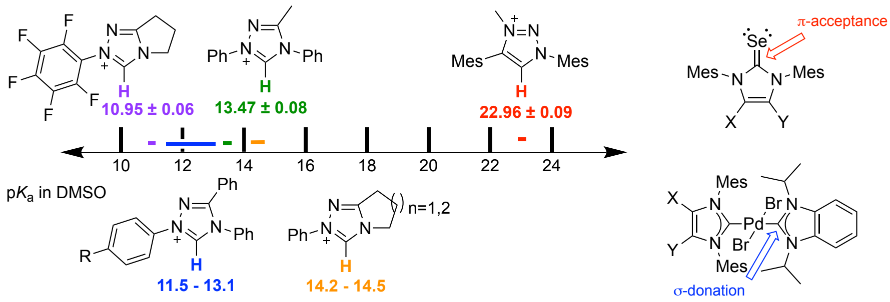
The project would involve kinetic analyses using NMR spectroscopy to monitor the progress of reactions, along with synthetic organic and analytical chemistry. Importantly, it can be readily tailored to either the physical and analytical aspects, with the opportunity to focus on methods to measure interactions and molecular dynamics simulations, or the more synthetic aspects, by focussing on designing new ionic liquids, increasing reaction yield and optimising isolation. Either way, you will be designing solvents to get the reaction outcome you want!



A series of ^{1}H NMR spectra showing the progress of a reaction, particularly the consumption of the starting material (◆) and formation of the product (◆).

b) Catalysis using *N*-heterocyclic carbenes: understanding structure/activity relationships[2]

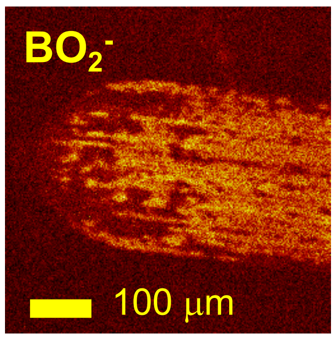
N-Heterocyclic carbenes, have significant roles in both organo- and organometallic catalysis, however some carbenes are effective for some processes but not for others; the origin of this is not well understood. This project aims to relate the structure and chemical properties of carbenes to catalytic efficacy; particularly the effects of changing steric and electronic properties will be assessed. Along with making the precursors to the carbenes, this project involves the opportunity to utilise various characterisation techniques (such as measuring acidity of parent cations to generating electronic probes based on Pd and Se) along with evaluation of catalytic systems; the latter can vary from screening of catalysts to detailed kinetic analyses. The ultimate goal is to be able to rationally choose an NHC catalyst for a given process.



The chemical properties of a carbene can be evaluated through the acidity of the corresponding salts (left, shown are triazolium salts) and the properties of selenium and palladium derivatives (right).

c) Broader applications of physical organic chemistry.[3] (collaborators include Drs Jeffrey Black, Jonathan Palmer, Chris Marjo and Prof. Chris Tierney, UNSW; Prof. Larry Scott, Boston College; Prof.'s Sergei Glavatskih and Mark Rutland, KTH, Stockholm)

The understanding developed above can be applied broadly – from understanding lubrication mechanisms to develop new compounds for mechanical engineering, through the synthesis of carbon nanostructures, to the preparation of samples to evaluate ancient climates. These projects focus on the ability to transfer understanding from one context to another and the skill sets required vary dramatically between projects. However, they all would suit someone with an interest in combining chemistry with an outside discipline as there will be opportunities to work closely with collaborators in different fields. Ultimately, these projects seek to expand the impact of the knowledge gained through our fundamental research.



ToF-SIMS analysis showing the breakdown products of an orthorborate ionic liquid in a wear scar after a lubrication test.

For more information, visit the group website at www.jasonbharper.com

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

1. A. Y. Hsieh *et al.*, *J. Org. Chem.* **2024**, *84*, 6427 & 14929; *RSC Adv.* **2023**, *13*, 21035; D. C. Morris *et al.* *ChemPlusChem* **2023**, e202300015; *Phys. Chem. Chem. Phys.* **2021**, *23*, 9878; M. D. Coney *et al.*, *J. Org. Chem.* **2022**, 833, 1767; A. Gilbert *et al.*, *J. Phys. Org. Chem.* **2021**, *34*, e3217; *Org. Biomol. Chem.* **2020**, *1*, 5442; **2019**, *17*, 675 & 9336; J. B. Harper *et al.*, *Phys. Chem. Chem. Phys.* **2021**, *23*, 2742 & **2020**, *22*, 23009; K. T.-C. Liu *et al.*, *Org. Biomol. Chem.* **2020**, *18*, 7388. For a review see *Adv. Phys. Org. Chem.* **2018**, *52*, 49.
2. C. Barnett *et al.*, *ChemistrySelect*, **2022**, *7*, e202104348; *Eur. J. Inorg. Chem.* **2021**, *47*, 4954; *Chem. Method.* **2021**, *1*, 374; N. Konstandaras *et al.*, *Org. Biomol. Chem.* **2020**, *18*, 66 & 1910; M. H. Dunn *et al.*, *J. Org. Chem.* **2017**, *82*, 7324.
3. J. J. Black *et al.*, *Sci. Rep.* **2022**, *11*, 24021; P. Rohlmann *et al.*, *Tribol. Int.* **2023**, *181*, 108263; **2021**, *161*, 107075; S. A. P. Blake *et al.*, *Dendrochronologia* **2020**, *60*, 125644; X. Zheng *et al.*, *Mires and Peat*, **2019**, *24*, 30; S. R. D. George *et al.*, *Polycycl. Arom. Compd.* **2016**, *36*, 897; *Org. Biomol. Chem.* **2015**, *13*, 9035 & 10745.

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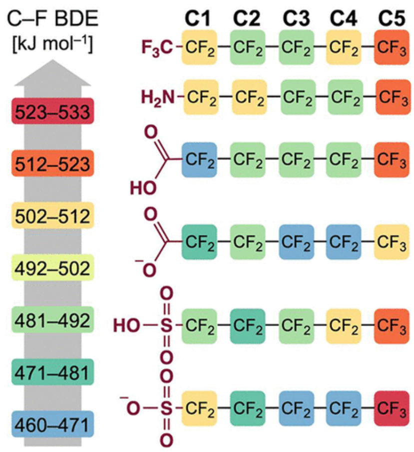
COMPUTATIONAL CHEMISTRY AND BIOMOLECULAR SIMULATIONS

We develop and apply computational chemistry methods to elucidate the mechanisms underlying many processes in synthesis and in biology (https://sites.google.com/view/mmg-unsw/home). This insight enables us to rationally design improved chemical reagents, drug molecules and materials that our experimental colleagues can test or implement in practical applications. Topics of particular interest include, but are not limited to drug design, solvent effects and supramolecular chemistry. We work closely with experimental groups at UNSW 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 first year chemistry is assumed and training and access to scripting and supercomputing resources will be provided.

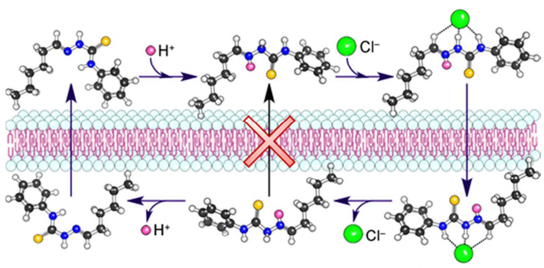
(a) Safe alternatives to "forever chemicals" – perfluoroalkyl substances (PFAS)

Perfluoroalkyl substances (or PFAS) are used in food packaging materials, fire fighting foams, fabric coatings and even some cosmetic products because of their extreme chemical and physical stability.[1] They are sometimes called "forever chemicals" as it takes a very long time for them to breakdown in the environment. Of concern, these molecules have been found to bind very strongly with the proteins and enzymes in our bodies[2] and some of them are classified as Class I carcinogens. It is therefore imperative that chemists and material scientists develop alternative materials that can replace PFAS and limit human exposure. This Honours project aims to use quantum and classical simulations to understand how fluorination gives rise to their water and grease-repelling properties (i.e. "amphiphobicity") and use that insight to propose environmentally-friendly alternatives.



(b) Anionophores as novel anti-cancer agents

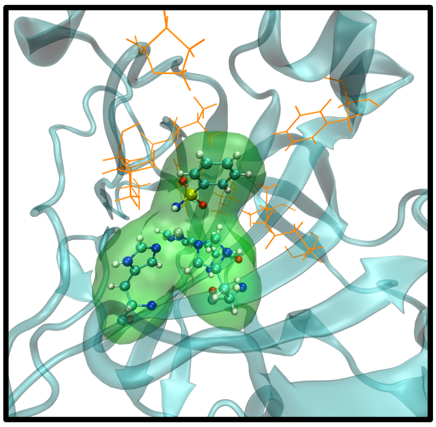
Anionophores are molecules that bind anions, most commonly through hydrogen bonding. Recent studies have revealed that these molecules can also perturb the ionic gradient in cells by transporting anions across cell membranes thereby leading to cell death (see for example, *Nature Chemistry* **2017**, *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 determine the free energy barriers for the transport of a ligand across the cell membrane. This will help establish the



important design principles for the development of more effective anion transporters. The tools developed as part of this project will also support efforts to predict membrane permeability of drug-like molecules in other applications.

(c) Simple models to predict blood brain barrier permeability of small drug-like molecules

Many enzymes exist in different forms that perform different biological functions. Selective targeting of specific isoforms is crucial for drug potency and minimising side-effects. The carbonic anhydrase enzyme has important regulatory functions and there are 15 known isoforms in human; two of which are associated with tumour progression (CA XI and CA XII). In this project, we will develop highly accurate multi-scale computational models to elucidate the molecular interactions that give rise to selectivity towards different isoforms of carbonic anhydrase. This insight will be crucial for the development of next generation CA inhibitors with greater selectivity. (Right: crystal structure of a CA inhibitor in the enzyme active site). The student will learn advanced techniques such as molecular dynamics simulations and quantum mechanics/molecular mechanics (QM/MM) methods.[3]



(d) Accelerating quantum chemistry calculations

One of the key achievements in modern quantum chemistry is the development of theoretical methods that can predict the behaviour and properties of molecules with accuracy that can rival experiments. However, the computational cost of these methods is so high that they are limited to very small molecules and chemists are forced to use less reliable methods to treat larger and more realistic reactions. Our group has a track record of developing efficient methods that help expand the scope of these rigorous theoretical methods to larger systems.[4,5,6] For example, we recently shown that is possible to accurately approximate the energies of very large water clusters (~ 200 atoms) by performing much smaller and therefore computationally tractable subsystem calculations using many-body methods. In this Honours project, the student will develop and implement an automated algorithm that will enable chemists to make fast and reasonably accurate estimates of the energies and vibrational frequencies of large molecular systems such as DNA quadruplexes. This project would suit a student with a strong interest in theoretical chemistry, analysis and coding.

$$E = \sum_{i=1}^{N} E_i + \sum_{ij} \Delta E_{ij} + \sum_{ijk} \Delta E_{ijk} + ...$$

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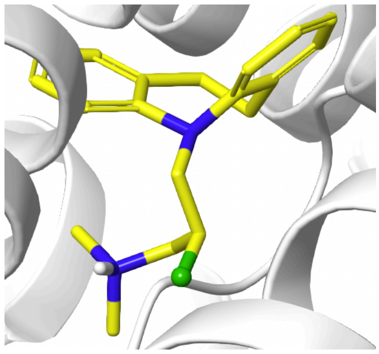
MEDICINAL ORGANIC CHEMISTRY

In my lab, we seek to make molecules that can treat disease. Our work relies on synthetic organic chemistry as the foundational activity, but we also employ a variety of other techniques such as molecular modelling, docking, NMR-based conformational analysis, solid-phase peptide synthesis, and many types of bioassays. Much of our work is highly collaborative in nature, and my students frequently spend time in other labs across UNSW as part of their studies. The broad project areas described below are constantly evolving, and I hope that the descriptions will serve as the *starting point* for a conversation with you about an ideal project that best suits your interests.

(a) "Molecular origami": using fluorine to control the shapes of bioactive molecules

(in collaboration with Dr. Junming Ho; Dr. Angela Finch [SOMS]; Dr. Nicola Smith [SOMS])

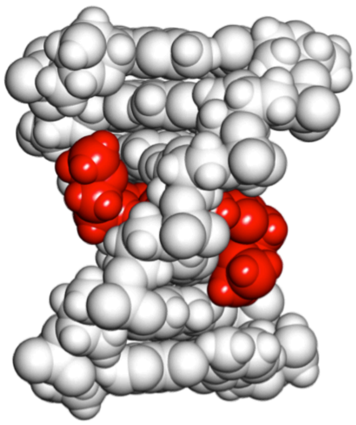
Fluorine is a small atom that packs a big punch. When incorporated into an organic molecule, fluorine can have a dramatic impact on molecular properties such as pK_a, metabolic stability, 3D conformation, and binding affinity for protein targets. We like to take conformationally flexible lead compounds, and decorate them with carefully designed patterns of fluorine atoms.[1–6] This can pre-organise the molecule into the target-binding conformation, thereby enhancing the biological potency and selectivity. In this project, we will apply this concept to the antidepressant drug, imipramine.



(b) "Molecular Velcro": targeting DNA to treat brain cancer

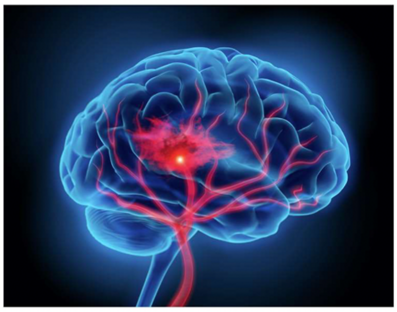
(in collaboration with A/Prof. Larry Wakelin; A/Prof. Graham Ball; Prof. Martina Stenzel; Prof. Bill Denny [Auckland]; Dr. Euphemia Leung [Auckland])

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.



(c) A "molecular high-altitude chamber": activating the hypoxia response to treat stroke
(in collaboration with Dr. Nicole Jones [SOMS]; Prof. Christopher Schofield [Oxford])

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, which will put nerve cells into damage-control mode after a stroke.[7] The key is a molecular-level understanding of the proteins that naturally activate this hypoxia response.



(d) A "molecular production line": new ways to synthesise ^{18}F-labelled compounds
(in collaboration with A/Prof. Giancarlo Pascali; Dr. Ben Fraser [ANSTO])

^{18}F-Labelled compounds are useful tools for PET imaging. We're pursuing efficient new methods for synthesising such compounds, including the use of flow chemistry, electrochemistry and photochemistry. We're also seeking to broaden the variety of ^{18}F-labelled compounds that are available in the clinic. For example, the pentafluorosulfanyl (SF_5) group can be considered as a "super CF_3 group," and it promises to deliver valuable future opportunities in medicinal chemistry and imaging applications.[8]

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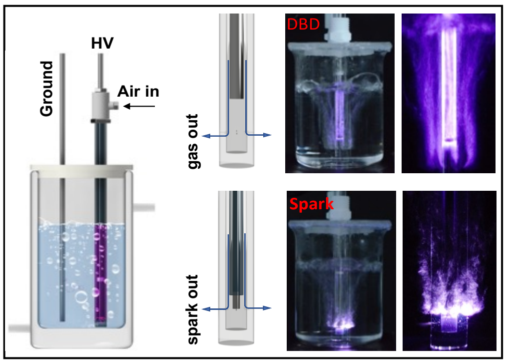
PLASMA, 3D PRINTING, AND ELECTRIFICATION FOR SUSTAINABILITY

My research group is focused on plasma science and technology and sustainable practices to develop practical solutions to environmental challenges. In accordance with net-zero emission objectives, our research concentrates on the development of green hydrogen technologies, decentralised fertiliser systems, and green ammonia production, which includes transportation solutions. We operate at the intersection of chemistry, physics, and materials science, advancing research in plasma catalysis, electrocatalysis, additive manufacturing, and advanced materials. Through a blend of academic study and industry-oriented initiatives, we aim to translate scientific findings into solutions with meaningful environmental and socioeconomic impact. We welcome undergraduate, Honours, and PhD students to engage in multidisciplinary projects and industry-related activities, offering hands-on experience with pilot systems, plasma processes, and sustainable energy technologies. Our group provides a unique opportunity to contribute to fundamental research while building expertise at the interface of science and industry.

Our projects will equip students with highly sought-after skills by industries navigating the growing demand for sustainable solutions. As industries increasingly turn to academia for innovative technologies, participants will gain practical experience bridging research and industry needs. Emphasis will be placed on scientific communication and collaboration to foster productive partnerships, aligning students with the evolving trend of innovation driven by societal demands, government incentives, and new business opportunities. This experience will position students for success in renewable energy and chemical industries, where they can generate impact with cutting-edge technologies.

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

(a) Plasma Gas Conversion for Value-Added Products



This project aligns with sustainable energy goals and offers practical insights into the application of plasma technology in renewable industries. Students will also gain experience working on innovative solutions that support the development of decentralised production systems. This project offers undergraduate and Honors students an exciting opportunity to explore the plasma-based conversion of gases such as nitrogen, air, methane, hydrogen, and CO_2 into value-added products. It focuses on reactor design, optimisation, and efficiency improvements. Students will experiment with various plasma reactor configurations, including non-thermal plasmas, which allow precise control over energy input and minimise losses through efficient ionisation. Using experimental and in-process simulation and multi-modal discharge reactors will enable students to explore different energy pathways and optimise plasma conditions to enhance productivity.

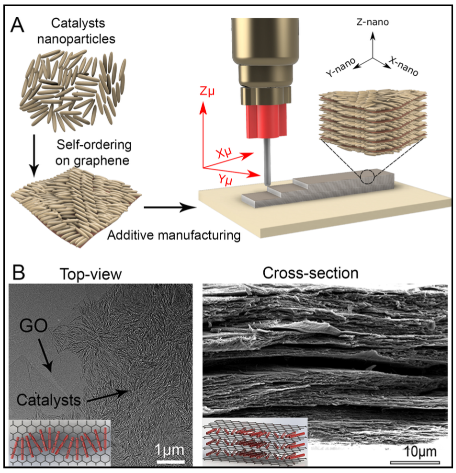
(b) Electrocatalysis for Green Ammonia and Fertiliser Production

This project offers a unique opportunity to engage in cutting-edge research at the intersection of advanced material synthesis, nanocatalysis, and electrochemistry for sustainable chemical production. The primary focus is optimising the electrocatalytic reduction of plasma-generated nitrogen species from air to produce value-added chemicals, such as ammonia, urea and nitrates, under mild and energy-efficient conditions. Students will develop, synthesise, and test nanostructured catalysts to enhance reaction selectivity and efficiency, driving progress in decarbonisation and sustainable chemical processes.

Throughout the project, students will gain valuable hands-on experience with essential research skills, including electrocatalysis, advanced material synthesis, and electrochemistry. Participants will also develop expertise in material characterisation techniques such as microscopy (SEM, TEM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and the operation of electrochemical cells and electrolysers. Additionally, they will explore computational modelling tools to predict reactions and optimise catalyst performance. They will be well-equipped for careers in emerging fields, seizing early opportunities driven by evolving government and corporate priorities, including net-zero targets, sustainability initiatives, and the transition to renewable energy solutions.

(c) 3D Printing and Biomimetic Liquid Crystal Scaffolds

This project allows students to explore the convergence of 3D printing, electrocatalysis, and advanced materials for sustainable chemical production. The focus is developing high-performance catalysts using nanomaterials such as nanofibers, nanotube nanoparticles, liquid metal alloys, and a wide range of two-dimensional (2D) semiconductors, including graphene and MoS_2. Students will fabricate scaffold electrodes by leveraging the self-assembly and liquid crystalline properties of 2D materials like graphene to fine-tune nanoscale interactions while controlling macro-scale structures through 3D printing techniques.



The project aims to advance the use of these functional scaffolds for both electrocatalysis and plasma catalysis, creating efficient systems for processes like gas conversion and synthesis. Students will design, fabricate, and characterise these advanced structures, gaining hands-on experience in material synthesis, 3D printing, and catalyst optimisation. This interdisciplinary work prepares students for careers in emerging fields focused on sustainable energy, materials science, and additive manufacturing.

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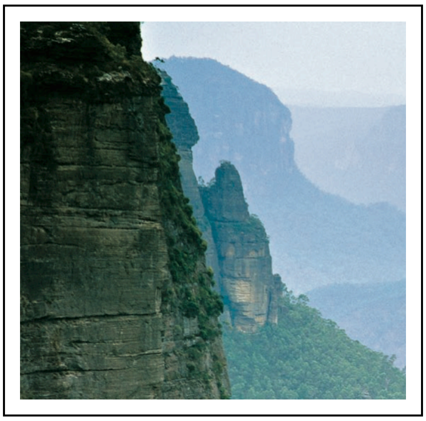
LASER PROBES OF CHEMICAL REACTIONS

- Use lasers to initiate photochemical reactions of relevance to atmospheric chemistry;
- Discover new chemical reaction mechanisms that cannot be explained by current theories;
- Discover new radicals using laser spectroscopy.

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

(a) The Atmosphere is on Fire!

(Collaborators: Meredith Jordan, USyd.; Jenny Fisher, James Cook U; Chris Hansen, UNSW)



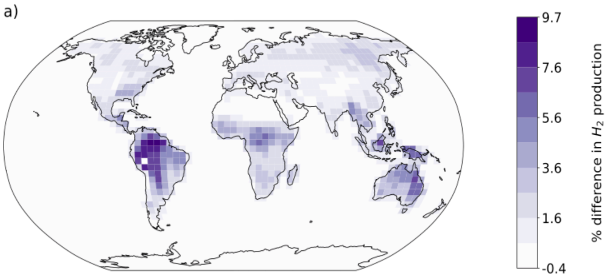
The poor state of our atmosphere is one of the most pressing issues facing society today. Everyone knows about the challenges of climate change. But did you realise that more people meet premature deaths from poor air quality than form either cancer or heart disease?

The chemical complexity of the atmosphere is extreme. More than 1 million organic molecules are suspected to be in the air. Add to the mix, solid and liquid aerosols, sunlight, and a range of pressure and temperature and you might understand the challenge in creating a model of our atmosphere that is accurate and predictive. Fundamentally, models are only as good as the underlying chemistry that they contain.

Our contribution in this area is in the discovery of new chemical mechanisms. Not just a new reaction, but new <u>classes</u> of reaction that are relevant across large domains of atmospheric science. Our latest project is built on our discovery in the past 2 years of light-induced combustion reactions. Organic molecules react with O_2 in a combustion environment because of the high temperature. This is an equilibrium environment where molecules are characterized by a temperature. But we discovered that organic molecules can absorb light and undergo combustion reactions in the atmosphere. Sunlight is acting like the match to induce these new reactions.

Your project can be experimental, computational, or modelling-based or any mix of the three. In the lab, you can use laser-based techniques to characterize light-initiated combustion in one target molecule. Computationally, you can determine the critical reaction pathways and critical energies for a number of target molecules and predict which will react and which will not. Using sophisticated atmospheric models, you can predict the impact of these new reactions on our understanding of atmospheric processes (see figure at left).

a)

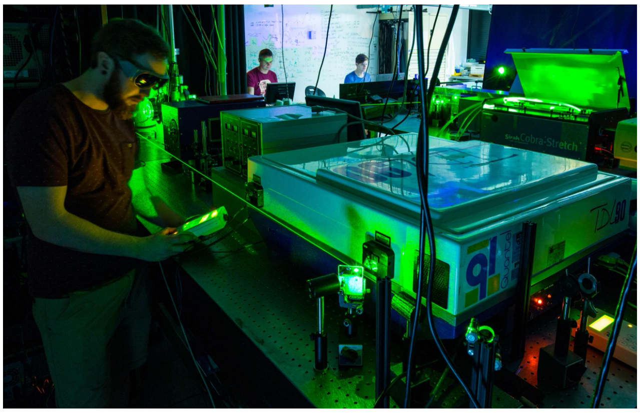


(b) Weird chemistry – reactions that just don't go where they should. (Collaborators: Meredith Jordan, Sydney U., David Osborn, Sandia National Labs, USA)

Since the 1930's, the concept of a transition state (TS) has formed the bedrock of chemical reaction theor[1]y. 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 new, unexpected products. Roaming has been described as the most important new fundamental reaction class discovered in the past 20 years and new aspects of how roaming works are still being discovered.

This project will explore quantum resonances in roaming. We are trying to learn how quantum aspects, such as interference and resonance, influence roaming outcomes. The project would suit a student with a strong background in physics and can be experimental or computational (or both) in nature. For a longer description of the chemical physics of this reaction have a look at this video:



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

Free radicals are key intermediates in all complex chemical environments. OH radical attack is the first step in the "processing" of nearly all atmospheric compounds. Radicals are found all through the interstellar medium and propagate flame chemistry. Of course you cannot buy a bottle of radicals form Aldrich (!) so you have to make them *in situ* and study them before they react with anything.

This is an inherently spectroscopic project where radicals are made in a vacuum using a variety of methods in our lab. They are characterised by a suite of spectroscopic techniques to determine their structure and chemical properties. Many times, you would be "seeing" a chemical species never seen before.

This project will involve the formation, measurement and characterization of a radical, chosen depending on your interest (space, combustion, atmosphere). A variety of laser spectroscopy techniques will be used to measure its properties. In concert with computational methods the structure of the radical can be worked out in fine detail.

[1] https://www.dropbox.com/s/ai9y1vyti3no8b9/Science_marketing_compressed2.mp4?dl=0

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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) Directing the chemistry/architecture of 3D extruded soft biomaterials

3D printing of cells and tissues is limited by issues with complex bioink formulation, segregation of different cell types, cell viability during prolonged printing, and difficulty recreating complex architectures observed in nature. New methodologies to quickly fabricate cell-laden tissue structures with well-defined segregated populations has the potential to be transformational to tissue engineering. We are exploring the extrusion of multiple hydrogel materials of tissue-mimetic composition (Fig. 1; *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.

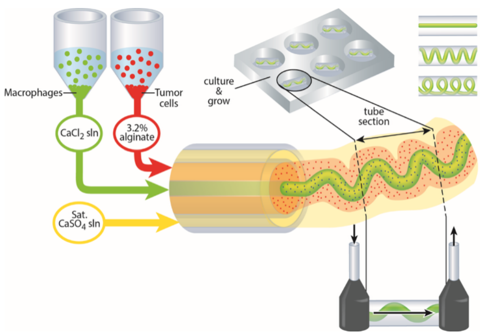

Fig. 1. Extrusion of cell-laden chemically modified alginate (*Adv. Mater., 2015*)

(c) Ceramic Omnidirectional Bioprinting in Cell-laden Suspensions (COBICS)

The integration of hierarchical structure, chemistry, and functional activity is important for building bone mimics for tissue engineering. Bone is a highly mineralized tissue with an organic matrix cotaining bone residing cells. Inspired by bone biomineralization, we have developed a novel apatite-transforming ink that can be

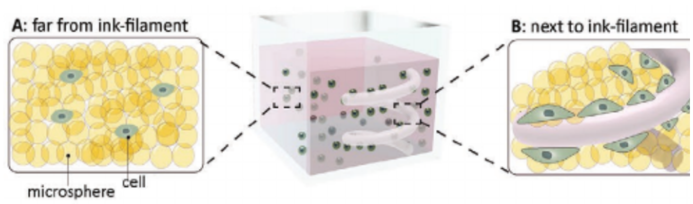

Fig. 2. Ceramic Omnidirectional Bioprinting in Cell Suspensions (Romanazzo et al., *Adv. Funct. Mater.*, 2021)

printed into a supportive microgel matrix with living cells (Figure 2; Adv. Funct. Mater. 2021). Using this technique, complex bone-mimicked constructs are made at room temperature without requiring invasive chemicals or high temperatures. This new strategy for fabrication of synthetic bone has scope for creating custom microenvironments for disease modeling and 3D printing bone directly into a patient. We currently have projects exploring new ink formulations to modify the inorganic and organic part to improve printability and healing.

(d) Synthetic tumours for cancer nanomedicine development

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 3; 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.

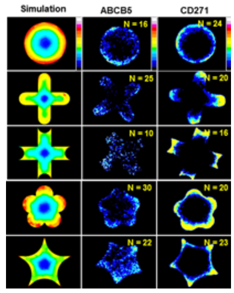

Fig. 3. Interfacial curvature will guide the activation of a stem-like state (Lee et al., *Nat. Mater.*, 2016)

Bringing mechanochemical activity to hydrogels

Hydrogels in tissue are viscoelastic materials that are continuously remodelled, and undergo dynamic changes in chemistry. Recreating dynamic chemistry in the laboratory most often involves incorporation of stimuli-responsive motifs, or secondary polymerization routines. We are investigating chemical linkages in hydrogels that are dynamic in response to stimuli including: temperature, pH, enzymatic activity and force. We are particularly interested in approaches where the chemistry can be modulated through applied compression or tension. Recently, we synthesised mechanophores that are "flex-activated" and demonstrated how compression and tension will trigger a retro Diels-Alder reaction to stimulate molecule release double network hydrogels (Fig. 4; *Chem. Commun. 2021*). We are looking for honours students interested in synthetic chemistry and polymer science to build the next generations of molecule releasing hydrogels for use as dynamic coatings and scaffolds for biotechnology and tissue engineering.

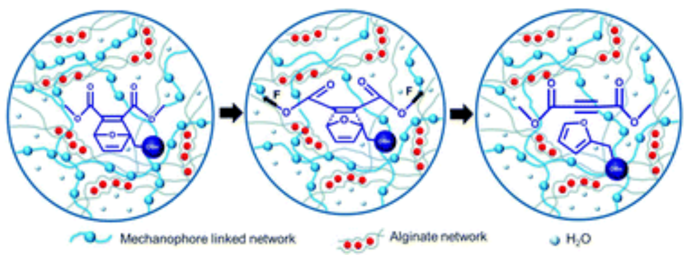

Fig. 4. Compression or tension triggers molecule release in double network hydrogels (Jayathilaka et al., Chem. Commun. 2021)

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.

DR. DONG JUN KIM

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SUPRAMOLECULAR ENERGY MATERIALS CHEMISTRY

We are a young research group which focuses on developing next-generation energy storages and supramolecular chemistry 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

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. Therefore, developing rechargeable batteries utilising aluminium offers a golden opportunity for delivering a high energy to cost per price. 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 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 chemistry and battery engineering. Based on the large selection and synthetic versatility of various organic molecules, the redox-active compounds based rechargeable Al-ion batteries could provide a promising starting point for developing affordable large-scale energy storage applications.

Rechargeable aluminium-ion batteries

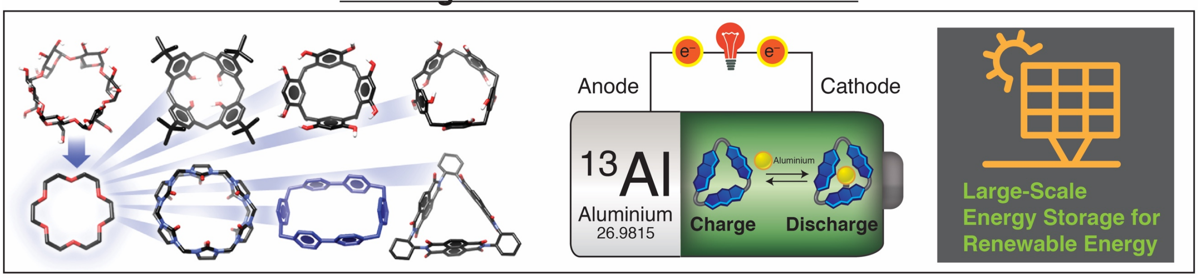

Figure 1. Graphical representation of the macrocyclic building blocks into nano-channels.

(b) Designing Molecular Dual Pump (in collaboration with Prof. Sir Fraser Stoddart in Northwestern University)

Artificial molecular machines have received an increasing amount of attention over the past few decades. They have the unique ability to generate directional motion of components within their molecules by energy inputs or external stimuli. In our group, we have developed chemically- and electrochemically-driven molecular pumps in order to trap cyclobis(paraquat-p-phenylene) ($CBPQT^{4+}$) rings on a collecting chain. A dual molecular pump can generate unidirectional motion along the dumbbell component using chemical reagents or electricity without accumulating waste products. By attaching a steric stopper at the end of the dual pump, the dumbbell will contain two collecting chains, making it possible to synthesize a [3]rotaxane sequentially.

This dumbbell consists of two pumps joined in series in a head-to-tail fashion with the first collecting chain located in the middle of them. It can be synthesized from the components that have already employed in the Stoddart Group. The second collecting chain is terminated by a bulky stopper. The target molecule will be produced using a click reaction.

Artificial molecular machines can be powered by chemical redox reactions where Zn (reductant) and $NOPF_6$ (oxidant) are used alternately. This in-series molecular dual pump can also be operated simply by the oscillation of two constant potentials (–0.7 V for reduction and 1.4 V for oxidation) in a controlled electrochemically powered process. The dumbbell contains two collecting chains which can accommodate at least two $CBPQT^{4+}$ rings. Heterotopic co-constitutional isomers of the [3]rotaxane could be generated by using $CBPQT^{4+}$ and a substituted $CBPQT^{4+}$ ring. By manipulating the pumping conditions with free and substituted $CBPQT^{4+}$ rings in the bulk solution, two different rings will be installed onto the dumbbell sequentially from the head to the tail.

<u>Artificial molecular dual pump</u>

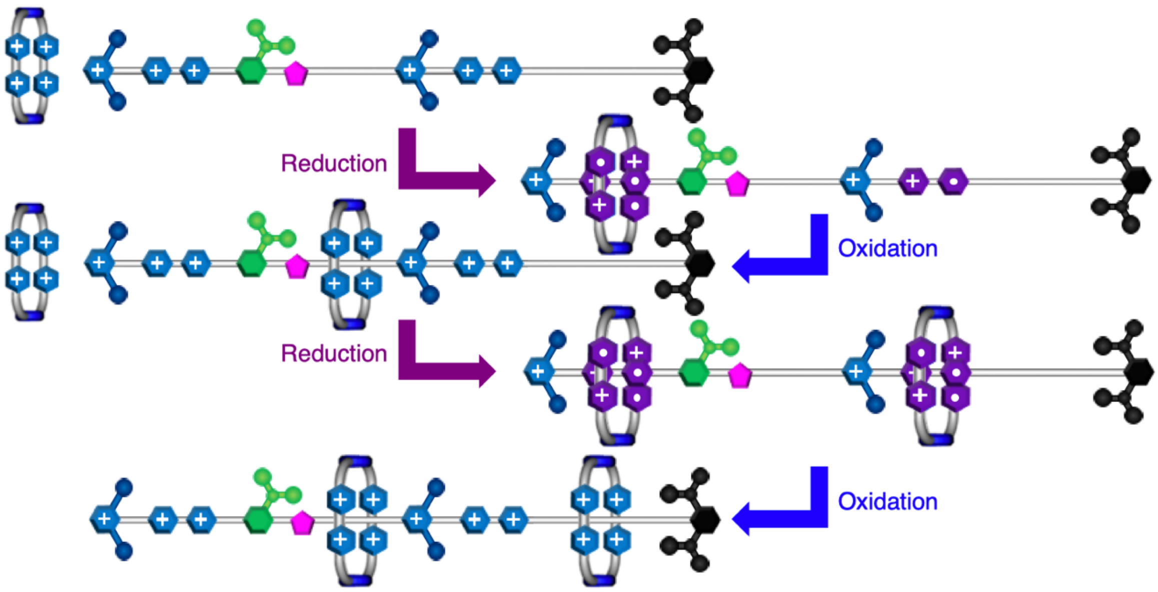

Figure 2. Structure the molecular dual pump and pumping rings onto the collecting chain chemically and electrochemically.

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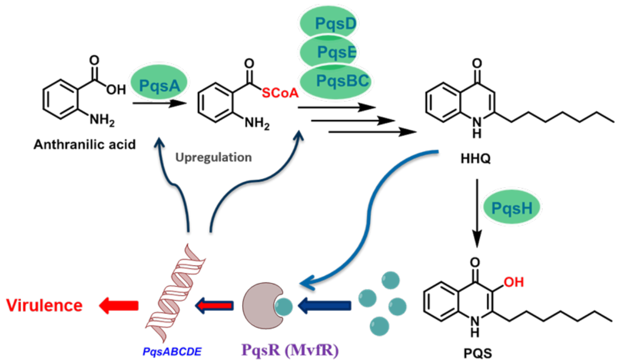
SYNTHETIC ORGANIC AND MEDICINAL CHEMISTRY

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

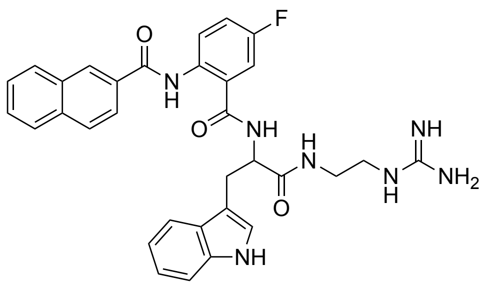
Quorum Sensing Inhibitors

(in collaboration with Dr Tsz Tin Yu, UNSW)



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.

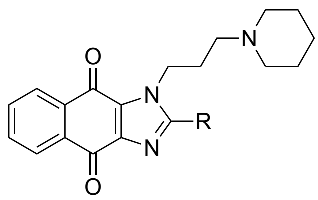
__Inhibitors of Bacterial Transcription Initiation__

(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 OXIDATION

(in collaboration with Dr Frances Byrne and A/Prof Kyle Hoehn, BABS, UNSW)

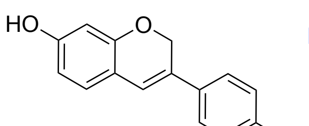


Cancer is a major burden of disease, affecting the lives of tens of millions on a global scale. A hallmark feature of nearly all cancer cells is their altered metabolism of glucose compared to non-cancerous cells. Relative to most normal cells, cancer cells use a greater proportion of incoming glucose 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.

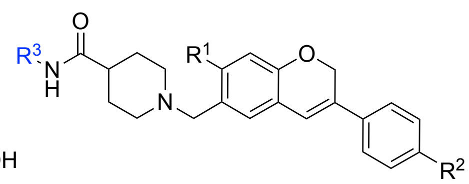
(c) DESIGN AND SYNTHESIS OF NOVEL INHIBITORS TARGETING ACUTE MYELOID LEUKEMIA

(in collaboration with Dr Daniel Wenholz UNSW)

Acute Myeloid Leukemia (AML) is a blood cancer (leukaemia) that represents ~40% of all new adult-onset leukemias in Australia. It is characterised by the overproduction of abnormal myeloblasts in the bone marrow, preventing healthy myeloblast, platelet and erythrocyte production. FMS-like tyrosine kinase 3 (FLT3) is a class III tyrosine kinase receptor involved in the regulation of hematopoietic cell differentiation, survival and proliferation. FLT3 mutations are among the most frequently identified mutations involved in leukaemia development and occur in approximately 28% of AML patients. Mutations of FLT3 have been associated with a poor prognosis, specifically adverse disease features, poor survival and a reduced rate of remission. A derivative of phenoxodiol has been identified as a screening hit compound for inhibition against FLT3 mutants. The overall aim of this project is to investigate the structure activity relationship on FLT3 through the synthesis of a library of novel analogues.



Phenoxodiol



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SCIENCE EDUCATION RESEARCH & SUSTAINABLE CHEMISTRY SYNTHESIS

The Kyne group's research is in two distinct areas: advancements in science education research and laboratory-based sustainable chemical synthesis. Through our research, we aim to contribute to a sustainable and equitable future.

Our science education research encompasses inclusive learning environments and assessments, data analytics and integrating sustainability in the curricula. We use mixed methods approaches, including course artefacts, observations, quantitative and qualitative data and analysis.

Our laboratory-based research centres on sustainable catalysis, including reaction design and mechanistic understanding. We undertake organic and organometallic synthesis, and use heteronuclear NMR spectroscopy, electrochemistry and X-ray crystallography for analysis.

Students with chemistry, education, social science and other backgrounds are welcome, as we believe diversity is key to tackling interdisciplinary challenges. There are opportunities to collaborate with other groups at UNSW, or across Australia and overseas.

Please feel free to contact me to discuss your own research interests and potential project ideas.

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

(a) Integrating sustainability and green chemistry into the chemistry curriculum

(in collaboration with Dr. Martin Peeks and Dr. Samantha Furfari, UNSW)

We aim to future-focus the curriculum to prepare undergraduate students to tackle global challenges confronting modern society. To achieve this, we are designing and implementing context-based learning activities that link fundamental chemistry concepts with modern society, using a systems thinking approach. Our goal is for students to use chemistry to develop multidisciplinary solutions to sustainability's "wicked problems". In addition to measures such as academic performance, student satisfaction and engagement, these activities are being evaluated based on impact on students' motivation and changes in perceptions towards sustainability as influenced by the enhanced curriculum.[1]

THE GLOBAL GOALS
For Sustainable Development

(b) Designing authentic assessment and feedback practices to enhance student learning

(in collaboration with the Australian Council for Educational Research)

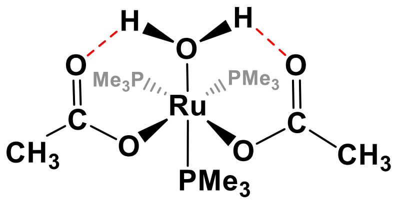
Assessment plays an important part in higher education and the student learning journey. Our research aims to change science assessment practices by creating and evaluating more effective and inclusive assessment strategies. In science disciplines, it is particularly important that assessment is authentic and relevant, ensuring that graduates are ready for employment. Our research focuses on improving how students' knowledge and skill attainment are assessed, and the quality of feedback that students receive. We do this by developing innovative assessment strategies that algin with real-world challenges to enhance student engagement and career aspirations. Our research aims to foster more inclusive assessment strategies to broaden participation, retention and diversity of science graduates.

(c) Developing inclusive chemistry learning environments

There is increasing diversity of learners in higher education with different backgrounds, and we are researching effective ways to create inclusive, accessible science learning environments for all students. We are designing proactive and flexible teaching approaches and learning resources, guided by the Universal Design for Learning framework.[2] To inform our approaches, we use data analytics to establish clear metrics to evaluate and improve inclusivity in chemistry teaching and learning environments.

(d) New ruthenium water complexes for catalytic hydrogenation

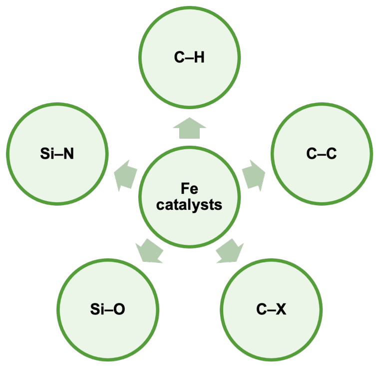
(in collaboration with Prof. Les Field, UNSW)



The Field group have recently discovered a series of ruthenium carboxylate complexes which strongly bind water. The carbonyls of the carboxylate ligands form a perfect pocket to bind a molecule of water with strong hydrogen bonds between the carbonyl oxygens and the water protons. These are remarkably stable metal complexes, and they are active catalysts for the homogeneous hydrogenation of simple alkenes. The project aims to improve and optimise the catalysts by: (i) modifying the molecular structure through variation of the ligands; (ii) investigating the mechanism for hydrogenation to inform catalyst optimisation; and (iii) tune the reduction conditions to optimise catalyst efficiency. We will also examine the potential reduction of other functional groups (such as esters, carboxylic acids, amides, nitriles etc).

(e) Developing new sustainable iron catalysed reactions

(in collaboration with Dr. Ruth Webster, University of Cambridge, UK)



First row transition metals are use as homogenous and heterogeneous catalysts that offer improved sustainability compared with precious metal catalysts. Iron can act as a powerful redox active catalyst for both single- and two- electron transfer processes, opening up a wide range of potential reactivities. We are designing new iron-based synthetic methods for applications including polymerisation and depolymerisation, intra- and intermolecular radical reactions, and main-group bond formations. Our research investigates the mechanism of the catalytic cycles, aiming to identify key reaction intermediates and understand chemical, physical and electronic properties impacting catalysis.[3]

1. Chen, A. Z., Peeks, M. D., & Kyne, S. H. (2025). *Journal of Chemical Education*, *102*(6), 2283–2293. https://doi.org/10.1021/acs.jchemed.4c01326
2. Reyes, C. T., Lawrie, G. A., Thompson, C. D., & Kyne, S. H. (2022). *Chemistry Education Research and Practice*, *23*(2), 385–407. https://doi.org/10.1039/D1RP00171J
3. Farcaş-Johnson, M. A., Gasperini, D., King, A. K., Mohan, S., Barrett, A. N., Lau, S., Mahon, M. F., Sarazin, Y., Kyne, S. H., & Webster, R. L. (2023). *Organometallics*, *42*(20), 3013–3024. https://doi.org/10.1021/acs.organomet.3c00339

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COMPUTATIONAL MATERIALS SCIENCE AND CHEMISTRY FOR SUSTAINABILITY APPLICATIONS

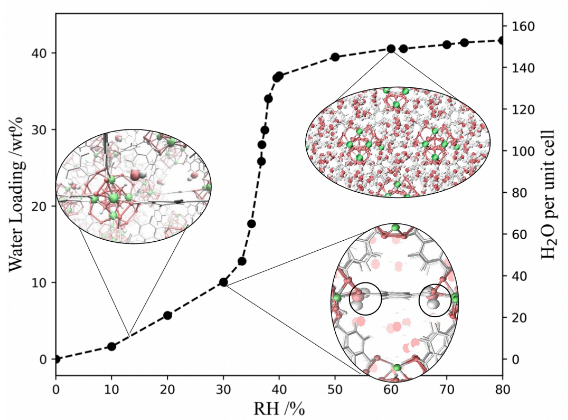
Computer simulations are an essential tool to make high-impact discoveries in fields that are crucial to our sustainable future. In general, these types of simulations allow us to calculate properties of molecules and materials at the atomic scale, which can be too difficult to be measured by experiments. 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 water purification and plastic recycling 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 Clean Water Harvesting and Water Purification

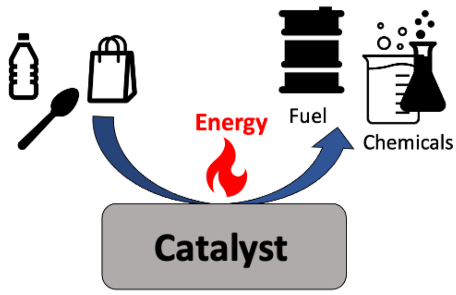
Access to clean water has been recognized as an essential human right by the United Nations. However, water contamination issues still exist and often render drinking water unsafe even in well developed countries. Developing cost-effective and efficient materials for clean water harvesting and polluted water treatment is necessary to ensure access to clean water for all. Metal-organic frameworks (MOFs) are promising materials for adsorption-based clean water 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. We use computational chemistry to aid the development of new materials based on MOFs for the adsorptive removal of heavy metals from water and for harvesting clean water from the air.

(b) Plastic Waste Conversion into Useful Products using Transition-Metal Catalysts

The conversion of plastic waste into monomers and other useful chemicals is a promising avenue towards addressing the plastic waste issue and reducing the use of non-renewable resources to generate such products. Recent experimental studies have shown that transition metal catalysts can be used to perform this conversion at moderate temperatures and with good product control. This project uses computational tools to design improved catalysts.

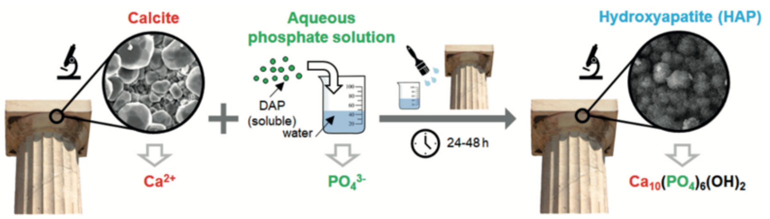


Overall we expect the results of these projects to guide experimental efforts towards the synthesis of improved and more cost-effective catalysts for plastic waste conversion into useful products.

(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.

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.



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

DR. LAUREN MACREADIE

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COORDINATION CHEMISTRY OF METAL-ORGANIC FRAMEWORKS

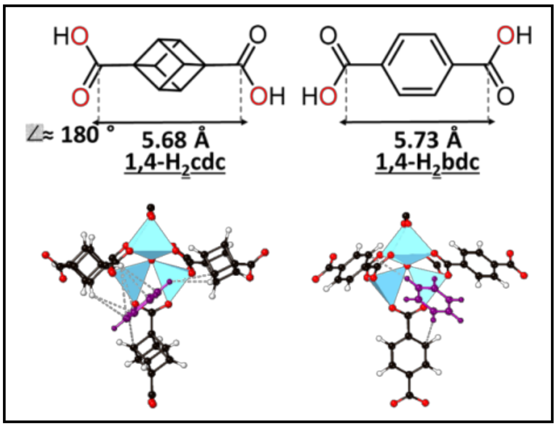
Metal-organic frameworks (MOFs) are porous coordination polymers built from the self-assembly of metal clusters and organic linkers. Through careful selection of these building blocks when designing our MOFs, materials with pre-determined properties can be synthesised. Our research area uniquely encompasses both organic and inorganic chemistry to develop interesting functional porous materials for catalytic hydrogen generation, gas storage and transport, negative thermal expansion and as MRI contrasting agents. Using diffraction methods from the Australian Synchrotron, we can piece together the structure-function relationships of these new materials and continually refine them for better performance.

Skills acquired from all projects include:

X-ray single crystal and powder diffraction, synchrotron science, MOF synthesis, organic and inorganic synthesis and characterisation using NMR, photophysical and gas adsorption…. Among many others!

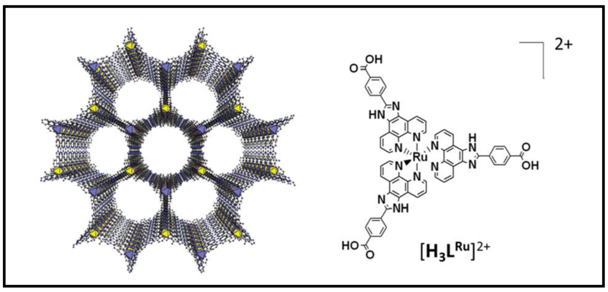
It would be fantastic to work with Honours students on the following projects:

(a) 3D-Linker MOFs for separations and storage



Most MOFs are constructed using aromatic linkers, such as terephthalic acid (H_2bdc), due to their low cost and well understood chemistry. Consequently, over 10,000 MOFs are made with only H_2bdc, giving a very poor representation of possible MOF environments. Our team works with rigid, 3D-linkers linkers such as cubane-1,4-dicarboxylic acid (H_2cdc) and have discovered enormous potential in these systems. Due to the bulky nature of the cubane, more supramolecular interactions are possible between the host and guest systems. This project extends the investigation to other 3D-linkers which will exhibit exciting properties. This high impact project and involves multiple collaborations, and investigates different factors governing host-guest behaviours. (Collaboration: Prof Omar Farha, Northwestern University, USA; and Dr Paul Savage, CSIRO)

(b) Photoactive frameworks for water splitting or CO_2 reduction

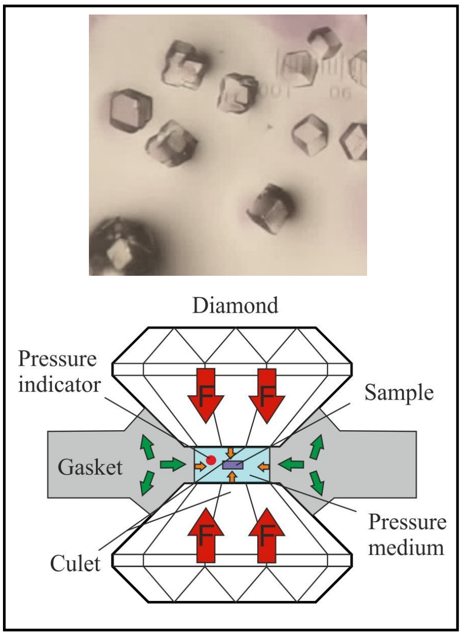


Luminescent MOFs (LMOFs) are rapidly gaining interest due to their promise in a broad range of applications including chemical sensing, artificial photosynthetic catalysis and optoelectronics. Recently, we have found tuneable luminescence can be gained through modulation of linkers

with mixed functionalities and the incorporation of mixed metals (eg. Ru and Co). This project investigates increasing the luminescent lifetimes of phenanthroline based MOFs through varying the conjugation in the MOF linker. As an added bonus, MOFs constructed from these linkers lead to large pores which are ideal for gas storage.
(Collaboration: Prof Lyall Hanton, University of Otago, New Zealand)

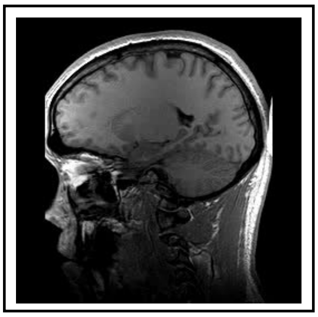
(c) Australian synchrotron high pressure X-ray diffraction to investigate negative thermal expansion (NTE) of 3D-Linker MOFs

Many materials exhibit positive thermal expansion with temperature. However, MOFs interestingly exhibit negative thermal expansion (NTE) – a phenomenon not often seen in materials. This is advantageous when trying to design zero thermal expansion materials which are highly sought after in industry. 3DL-MOFs exhibit enhanced NTE compared with aromatic frameworks due to the hyper-fast molecular rotor dynamics of the aliphatic cores. These rotor dynamics can be influenced by external pressure and temperature environments, further influencing the extent of NTE in these materials. This project will involve studying the response to external pressure of 3DL-MOFs through variable pressure and temperature X-ray diffraction studies run at the Australian Synchrotron using diamond anvil cells.
(Collaboration: Prof Cameron Kepert, University of Sydney; Prof. Stephen Moggach, UWA; Australian Synchrotron)



(d) NanoMOFs as dual MRI contrasting agents/drug delivery agents

The highly porous nature of MOFs allows them to hold and deliver large payloads such as drugs and nutrients. Furthermore, exploiting the coordination polymer nature of MOFs means that a high amount of MRI active agent can be generated in a nanosized material, which can be tailored to target specific sites in the body. NanoMOFs exhibit numerous properties which make them ideal for biomedical applications. Their highly porous structures allow accommodation of high loadings of therapeutic and imaging agents and their controlled release, in addition to protection against enzymatic degradation. This project investigates iron and gadolinium contrasting agents which can self-assemble to form NanoMOFs, and studies their controlled release at target sites in the body.



(d) Other projects for your interest including agriculture remediation and CO_2 capture!

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3. **Macreadie, L.K.**, Qazvini, O.T., Babarao, R. ***ACS Applied Materials & Interfaces***, *2021*, *13*, 26, 30885.

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COMPUTATIONAL MOLECULAR SPECTROSCOPY FOR ASTROCHEMISTRY AND BEYOND

Want to do research on a computer not in a lab? Feel constantly pulled between physics and chemistry? Love spectroscopy, quantum mechanics and energy levels? Or perhaps you want to utilise and strengthen your maths, programming and/or data science skills by exploring exciting molecular science applications from predicting 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.

Looking for life and its molecular origin in space

Keywords: *Computational Quantum Chemistry, Astronomy, Exoplanets, Spectroscopy, Supercomputers, Data Science, High Accuracy, High-throughput Calculations, Radio & Infrared Spectroscopy*

One of our group's key motivations is to predict spectral data that is immediately useful, often for characterising unusual astrophysical environments including exoplanets and the interstellar medium. Sometimes this means very high accuracy sub-cm^{-1} predictions of rovibronic spectra of weird diatomics like TiO, using all the experimental data we can find. Other times, this means producing approximate data for thousands of molecules to identify strong absorbers and molecules that will be difficult to distinguish astrophysically.

The primary purpose of the data is to enable astronomers to confidently detect molecules in various astrophysical environments. The highest profile of these sought detections are of course biosignatures in the solar system (e.g. phosphine on Venus) and exoplanets. Almost as important are the searches for the origins of homochirality and life through searches for pre-biotic and chiral molecules in the interstellar medium.

On a more local level, this type of generated data is important for monitoring atmospheric composition and pollutants on local and global scales and in industrial plants. It can also be used to predict global warming potential of different molecular compounds (e.g. those proposed as replacements for CFCs).

Machine Learning: Chemical Structure → Spectra

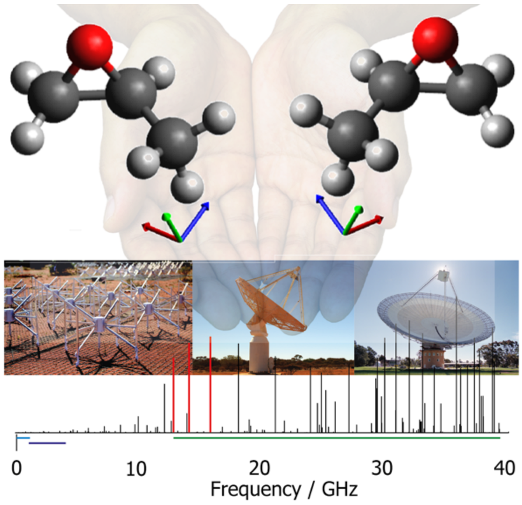
Keywords: Machine Learning, Data Science, Computational Quantum Chemistry, Supercomputers, High-throughput Calculations, Spectroscopy

Machine learning and "big data" science is starting to revolutionise many areas of chemistry, but one area hardly considered is spectroscopy. Can machine learning outperform quantum chemistry calculations in some (or all?) areas of modern computational molecular spectroscopy? The high-throughput data produced by my group provides a perfect training set for machine learning models to predict spectral properties from chemical structure without quantum chemistry, as a byproduct recreating organic chemistry infrared functional group tables.

Rotational Spectroscopy of Pre-biotic Chiral Species: Experiment & Theory (collaboration with Chris Medcraft)

Keywords: Astrochemistry, Experimental Spectroscopy, Computational Quantum chemistry

Why pick? Do a project that combines experimental rotational spectroscopy with computational quantum chemistry predictions, focused on the rotational spectroscopy of a pre-biotic chiral molecule that may help tell scientists how life emerged. This project produces crucial high-accuracy astronomical data required for the upcoming Square Kilometre Array radio telescope and its precursors.



Beyond this main body of work, other potential projects 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.

Finding 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.

Evaluating high-school outreach (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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SYNTHETIC AND MEDICINAL CHEMISTRY

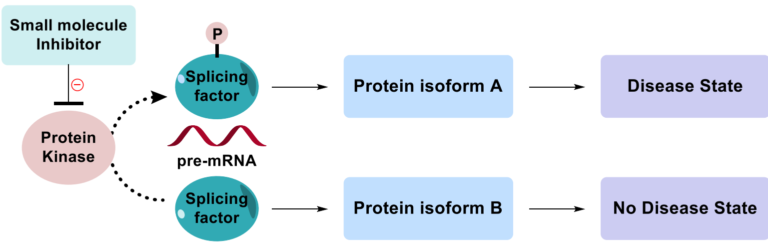
- The Morris group are focused on the development of organic molecules that can be used in biomedical research.
- They use their expertise in synthetic organic chemistry to access biologically active small molecules. Once an efficient strategy is developed, investigations into how these molecules interact with biological systems can be initiated.
- Being able to synthesise new small molecules in an efficient manner is critical and as such, the focus is on developing strategies to prepare these valuable materials and generate analogues that have improved potency and selectivity.
- Work on these areas leads to a number of collaborations with biomedical researchers where students can become involved in the understanding the biology.

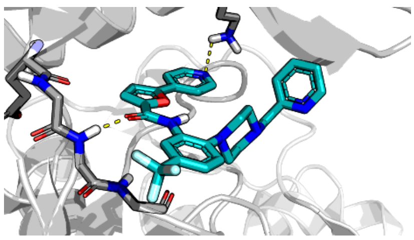
It would be great to work with Honours students on the following projects:

(a) Modulation of RNA splicing using small molecule kinase inhibitors

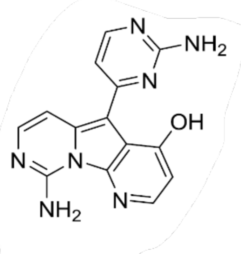
The control of the fundamental biological process of alternative RNA splicing is an emerging method for treating diseases such as aged macular degeneration and cancer. It has been established that by controlling the phosphorylation of key proteins in the spliceosome, it is possible to alter RNA splicing 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 of the splicing factors.

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 an eye drop treatment for aged macular degeneration in collaboration with Exonate. The recent phase 1b/2 clinical trial has confirmed that this strategy is therapeutically viable. This class of inhibitors have also been used by our biological collaborators at the University of Nottingham in their investigations into cancer biology and pain modulation.





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 further development of improved kinase inhibitors. A range of analogues have been developed that are more selective inhibitors of certain kinases, as well as have better properties such as solubility.

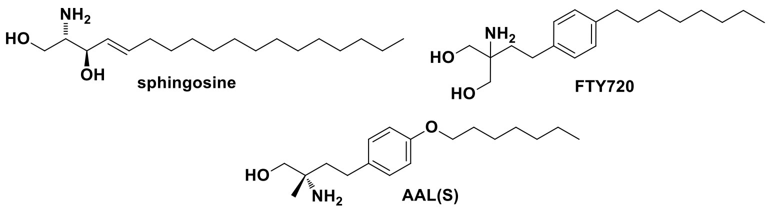


variolin B

Building on this work, we are engaged in the development of a number of different chemical scaffolds to inhibit the kinases that regulate alternative splicing. The aim is to develop selective inhibitors of the various RNA splicing 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.

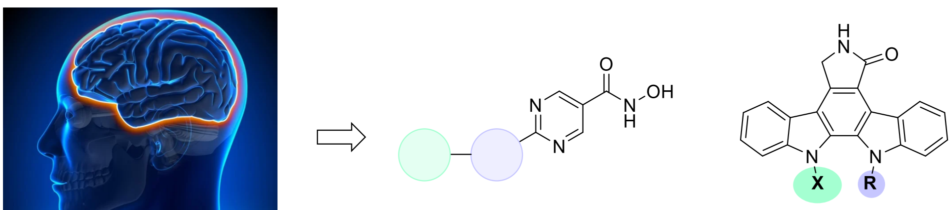
(b) Developing the AAL(S) Scaffold for Therapeutic Applications (with Prof Nigel Turner (Victor Chang CRI, UNSW Sydney), Prof Alaina Ammitt (UTS) and Dr Nikki Verrills (Newcastle)

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.



(c) Designing drugs that cross the blood-brain barrier to treat childhood cancers (with Prof Matt Dun (Newcastle))

Diffuse intrinsic pontine glioma (DIPG) is a highly aggressive brain tumour primarily affecting children. This disease is universally fatal, with critical location in brainstem ruling out surgical intervention. To date, there has been little progress made on developing therapeutics that target DIPG. One of the key challenges that arises is the inability of most small molecule drugs to cross the blood-brain barrier (BBB). Working with Prof Matt Dun (University of Newcatle) we are focussed on improving the brain-penetrant properties of potent anti-cancer drugs using a computer-aided multiparameter approach to predict which chemical changes will lead to improved permeability. Thus far we have demonstrated that simple chemical modifications can greatly improve BBB permeability while retaining anti-cancer activity. We are actively working on a series of chemical scaffolds that encompass a range of different synthetic approaches.



Brain-penetrant anti-tumor agents

(d) Disrupting the actin cytoskeleton to target breast cancer

Actin filaments are the structures responsible for the shape and locomotion of cells. While cellular migration is essential for biological processes such as tissue repair, uncontrolled migration is implicated in cancer cell migration and metastasis. Early actin-targeting therapeutics have struggled with selectivity between healthy and cancerous cells leading to problems with toxicity. In this project, the Morris group are working in collaboration with Dr David Croucher and Dr Sharissa Latham (Garvan Institute of Medical Research) improving the drugs' potency and drug-like properties.

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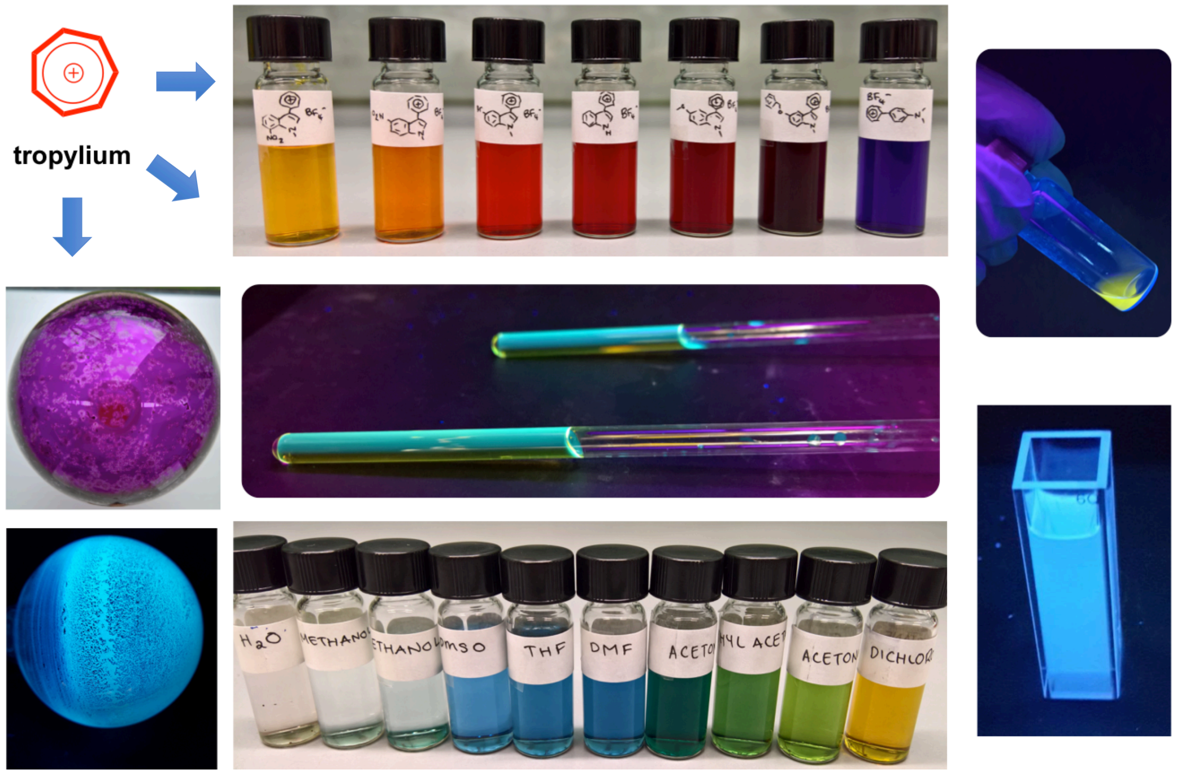
ORGANOCATALYSIS AND CHEMISTRY OF UNUSUAL MOLECULES

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.

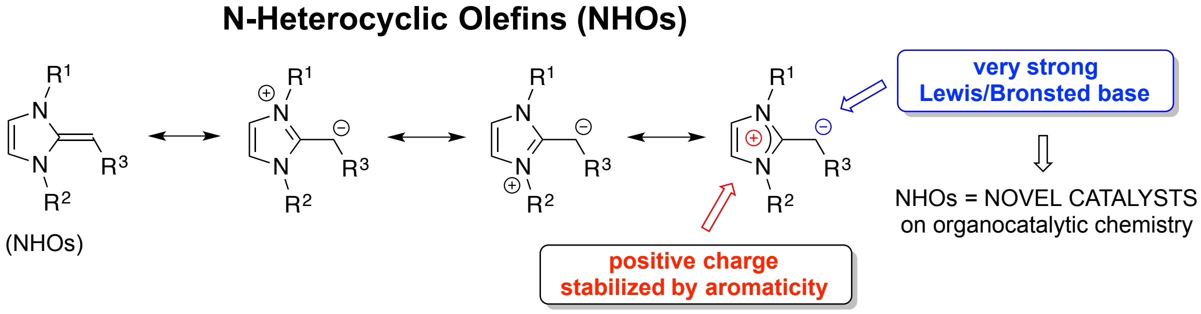
(a) Project NTV1 - Tropylium Ion as Chromophore for Organic Dyes

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.



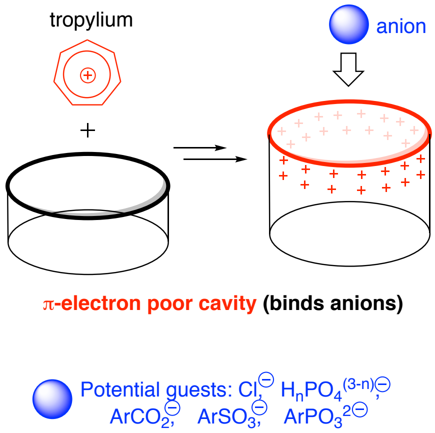
(b) Project NTV2 - *N-Heterocyclic Olefins as Novel Organocatalysts*

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 Prof Pall Thordarson)

This project will explore the potential of tropylium-bearing systems in host-guest chemistry in ***collaboration with 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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[2] **T. V. Nguyen**,* A. Bekensir, *Org. Lett.* **2014**, *16*, 1720-1723. http://dx.doi.org/10.1021/ol5003972

[3] **T. V. Nguyen**,* M. Hall, *Tetrahedron Lett.* **2014**, *55*, 6895-6898. http://dx.doi.org/10.1016/j.tetlet.2014.10.100

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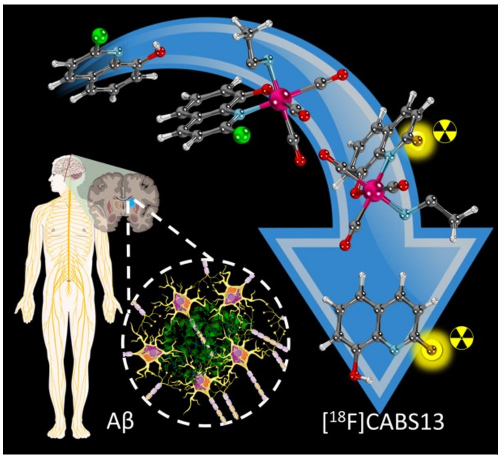
INNOVATIONS IN RADIOPHARMACEUTICALS AND RADIOCHEMICAL TECHNOLOGIES



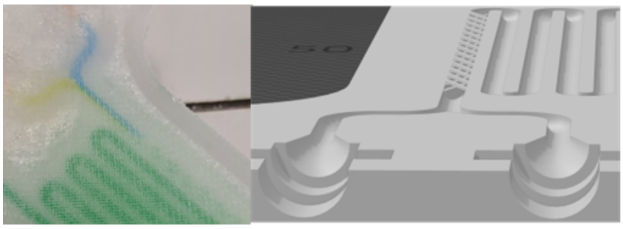
Credits: Dr. Mitch Klenner

Radiopharmaceuticals are becoming increasingly important for the management of many diseases, due to their extraordinary sensitivity and specificity. However, still many challenges are existent to deliver such high-value molecules, and they span from the initial molecular design, to efficient methods for radiolabelling and radioisotope purification, and to reliable process automation. Added to more standard radiopharmaceutical and radiolabelling development ideas, below are some examples of cross-disciplinary projects, that would anyway be tailored around student interests and desired skillset development.

(a) 3D-printed microfluidic reactors

(in collaboration with David Zahra, ANSTO)

Microfluidic systems have found multiple applications in the biochemical field, but are still not utilized extensively in the chemical reaction field. This is mostly due to the reduced availability of correct performance to be achieved for a chemical reaction (e.g. solvent resistance, pressure and temperature rating). However, new materials and advanced processes are now available for 3D-printing, and few works are demonstrating the feasibility of chemical reactions in microfluidic reactors manufactured in this way. In addition, it is demonstrated that radiolabelling reactions can happen with improved efficiency in the microfluidic environment; this fact, joined to the possibility of fast prototyping and single-use approaches (i.e. reduction of cross-contamination and radioactive waste), make 3D-printing of radiolabelling reactors a very attractive option. This project will explore this possibility, mainly using non-radioactive assessment, but ultimately testing the best results in model radioactive scenarios. The knowledge acquired can be translated in the development of other Lab-on-Chip systems.



Credits: David Zahra

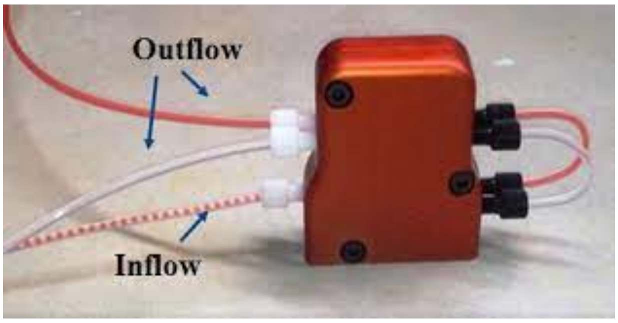
***Skills**: 3D-drawing software, 3D-printing equipment and process, functional test for microfluidic chips, instrumental analytical techniques (e.g. HPLC, GC), basics of CT imaging, basics of radiolabelling reactions.*

***Key reference**: FOMSy: 3D-printed flexible open-source microfluidic system and flow synthesis of PET-tracer; Journal of Flow Chemistry, 13, 247–256 (2023).*

(b) Separation of radioisotopes by liquid/liquid flow extraction

(in collaboration with Elisabeth Tondl, ANSTO)

The production of radioisotopes is the first step towards manufacturing radiopharmaceuticals. In many cases, it requires bombardment of a defined target material to induce the nuclear transformation, the separation of the desired radioisotope from the bulk target material, and its formulation into a form usable for successive radiolabelling steps. There is an ongoing need of novel and more efficient methods to achieve such processes, linked to the increasing clinical demand of radiopharmaceuticals. Traditional separation methods were based on liquid/liquid extraction (LLE); however, current industrial (and also research) methods are based on resin-based separation, due to its ease of automation. On the other hand, this approach typically features variability of resin batches and packing, use of large volumes of eluents (that need dedicated radioactive waste storage), and challenges in scaling-up. In recent years, few systems have become available that allows LLE to be performed at the continuous flow regimen, and with capability to be easily integrated in automated systems. Therefore, there is a substantial potential to revisit the traditional LLE methods in radioisotope separations, possibly leading to processes with improved separation efficiency, better chemicals control, reduced waste and easy scale-up. This project will assess this concept using non-radioactive chemicals and conditions that mimic real-life concentrations, and the most performing systems will be tested with radioactive mixtures from real-life bombardments. The knowledge acquired can be translated to the integration of online LLE in flow chemistry processes for other synthetic chemistry applications.



Credits: Zaiput Flow Technologies

***Skills**: Hydrometallurgy basics, synthesis and/or purification of ligands, flow chemistry concepts, unbiased optimization methods (DoE, ML, AI, algorithms), radioisotope separation basics.*

***Key reference**: Recovery of Gallium-68 and Zinc from HNO3-Based Solution by Liquid–Liquid Extraction with Arylamino Phosphonates; Molecules, 27, 8377 (2022).*

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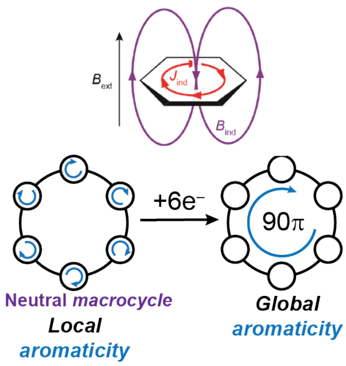
SUPRAMOLECULAR & ORGANIC MATERIALS CHEMISTRY

Our research is concerned with understanding the nature of electronic communication and conjugation and using these principles to make interesting new molecules and assemblies. In doing this we have two real goals: making molecules that have useful properties, and those 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:

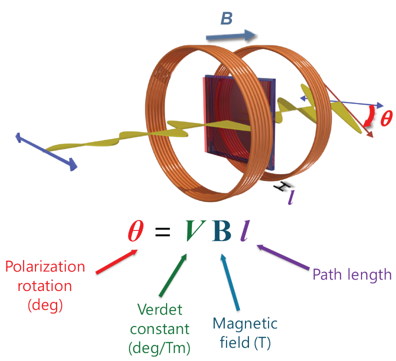
(a) Pushing the limits of π-conjugation, aromaticity, and antiaromaticity



π-conjugated molecules are like tiny little wires because they can delocalize electrons very effectively. Aromatic molecules are perhaps the archetypal π-conjugated molecules – things like benzene! They've been studied for more than 150 years, but much remains to be learned about aromatic and antiaromatic, as well as more unusual, molecules. For example, we recently reported the synthesis of the **largest known aromatic and antiaromatic molecules**.[1] In general we are interested in looking at new chemical structures which exhibit improved – or just unusual – π-electron delocalization and these are several projects available along these lines. We look at the effect of molecular structure on electronic delocalization and resulting properties like light emission and absorption (colour), wire-properties like electronic communication, and many more (see projects below).

Projects in this area span synthesis, analytical chemistry (NMR, optical spectroscopies), and computational chemistry – you can do whichever bits interest you most, or a bit of everything!

(b) Rational design of magneto-optic materials



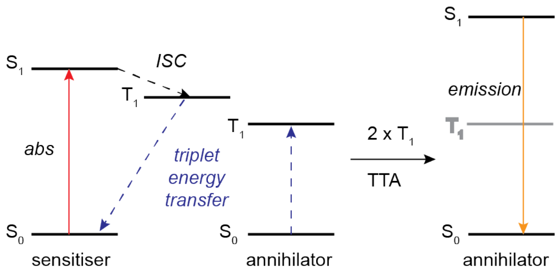
All transparent materials exhibit an effect called *magneto-optic rotation*, or *Faraday rotation*. This effect is quite important: it's used in photonic devices to control the propagation of light on very fast timescales, and could be used in next-generation magnetic-field sensors. Such materials would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

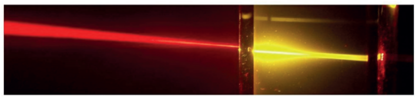
Despite the Faraday effect's ubiquity, it's actually quite weak in most materials, except some ferrimagnetic garnet materials – or that was the prevailing wisdom. Recently it's been discovered that a range of organic materials, from polymers through to liquid crystals, exhibit extreme Faraday rotation.[2] 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.

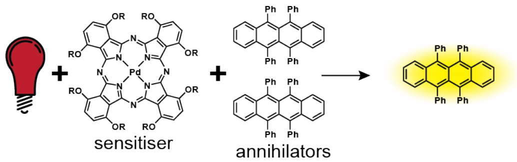
(c) Molecules and assemblies for photon upconversion (with Prof. T. Schmidt)

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.





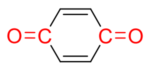
Picture from Schulze, Lips, Schmidt. Proc SPIE, 10.1117/2.1201403.005390



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]

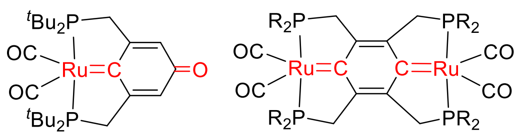
The project will involve synthesising a series of organic and inorganic chromophores to systematically explore structure-property relationships. There is an opportunity to use computational chemistry to predict molecular properties, and to measure your new materials in collaboration with the Schmidt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

(d) Metal-to-metal communication through cross-conjugated frameworks (with Prof Les Field)



p-quinone

Quinones are a class of organic compounds which have a rich redox-chemistry, and which are heavily used as oxidizing agents both by chemists and in biology. Metallaquinones are analogues of quinones where one or both of the oxygen atoms are replaced by metals. This project involves synthesising new bi-metallic or polymetallic quinonoid compounds and examining the redox chemistry and metal-to-metal electronic communication in this unusual class of molecules. The results provide fundamental insight into the nature of electronic communication and could underpin the design of the next generation of advanced materials.



metallaquinone dimetallaquinone

(e) 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!

1. P. Wang *et al. JACS* **2018**, 6501; P. Wang *et al. JACS*, **2018**, 10881; 2. M. D. Peeks, T. D. W. Claridge, H. L. Anderson *Nature* **2017**, *541*, 200; M. D. Peeks *et al. J. Phys. Chem. Lett.* **2019**, 2017; N. Toriumi *et al. JACS* **2015**, 82; 4. V. Gray *et al. Coord. Chem. Rev.* **2018**, *362*, 54.

DR. NICOLE J RIJS

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STRUCTURAL CHEMISTRY WITH MASS SPECTROMETRY & ION-MOBILITY

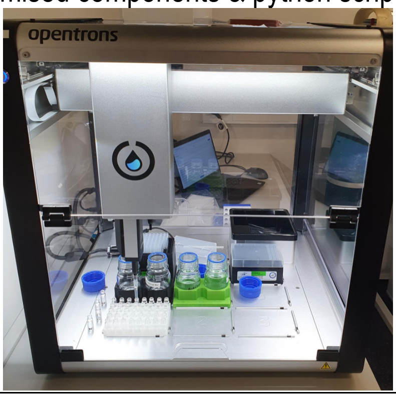
Can you envisage a world where building a new catalyst or an artificial enzyme is like following an architectural plan for building a house? This is difficult as we don't even fully understand the construction materials! We research the properties of molecular building-blocks and their "constructed" aggregates, towards drawing up these type of blueprints.

We use high resolution ion-mobility spectrometry and mass spectrometry, computational chemistry, combinatorial libraries and robotics; along with wet chemistry to understand structure and function. We are targeting many types of chemistry involving metal ions. The way we are currently using these techniques is unique.

Electrospray ionization-mass spectrometry (ESI-MS) is rapid, sensitive, precise and well-controlled. Ion mobility (IMS) separates **much quicker** than chromatographic techniques, in milliseconds rather than minutes or hours. It is ideal for measuring the size and shape of molecules and complexes.**[1]** It also seamlessly interfaces with mass spectrometry. We use these methods together to monitor target reactions, both simple and complex, with ease.

No prior experience required to get started with these techniques, but advanced MS skills such as these are currently in high demand in industry, with demand outstripping graduate supply.

A Our liquid handling robot, uses customised components & python script



By joining us, you can become expert at:

- different types of electrospray ionisation mass spectrometry & ion-mobility techniques
- robotic preparation and analysis (**A**),
- screening of chemical data sets,
- electronic computation, such as DFT
- collaborative projects with synthetic groups

Projects are tailored to your interests. We are interested in structure, structure-function relationships, mechanisms underpinning reactions, chemical data crunching and digitisation, and methodological development for mass spectrometry and ion-mobility. We are particularly interested in the way metals, ligands and organic molecules aggregate or react.

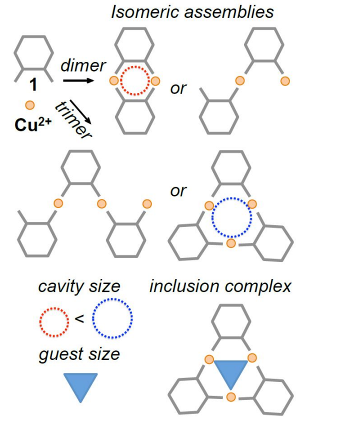
It would be great to work with students on the following projects:

Catching Structures within Dynamic Combinatorial Libraries

Dynamic combinatorial libraries are ensembles in equilibrium (as in **B**). Depending on the ligand, different shaped oligomers can assemble. This allows a high throughput screening for usefully shaped molecules.

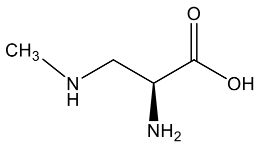
In this project, robotically generated libraries will be monitored for the evolving molecular assemblies. We will push the reactions using additives and other changes to solution conditions. These chemical investigations can pair with machine learning to increase output.**[2]**

B Dynamic library

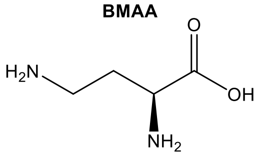


Assemblies of Relevance to Human Protection

C Non-protein amino acids & structural analogues



BMAA



2,4-DAB

From ubiqitous herbicides like glyphosate, to chemical warfare agents, to toxins produced by cyanobacteria, non-protein amino acids are significant. β-(N-methylamino)-L-alanine (BMAA) is commonly found in waterways in regional NSW due to algal blooms and has been implicated in ALS and Alzheimer's disease. One mechanism of toxicity is suggested to be due to its shuttling of metal ions to the brain.

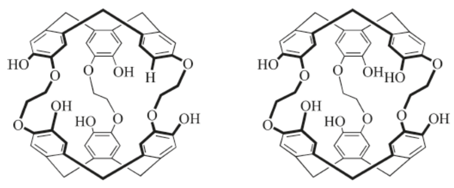
A combinatorial approach will be used to screen the metal complexes of BMAA and its structural analogue 2,4-diaminobutyric acid (2,4-DAB) (**C**) to learn how they behave dynamically and interact with metal ions.

Encapsulation Exquisitely Probed by Ion-Mobility

Cryptophanes (**D**) have extraordinary properties in water. They can capture methane or metal cations. They are targets for gas sensing, for environmental remediation of incredibly toxic thallium in water, and delivery of agents for MRI contrast.

In this project, the encapsulation properties of diverse cryptophane complexes will be investigate with the aim to tune them for their applications.

D Example cryptophanes



MM-1   *MM*-2

Clusters as Model Systems for Enzymatic Sites

Our ability to control chemical reactions is determined by the ability to observe them. Enzymatic reactions are notoriously difficult to observe. In this project, metals-ligand assemblies of urea, guanidine, formamide, & nucleobases will be analysed as well-defined models for enzymatic sites.

Antibiotics and the Significance of their Metal Complexes

Metal complexes of antibiotics are important, e.g. they may inactivate their mode of action, or be critical to steps in breaking down bacterial biofilms. In this project, the structures of metal complexes of antibiotics of global importance will be analysed to understand their role and underpinning mechanisms.

[1] Front. Chem., 2021, 9 DOI:10.3389/fchem.2021.682743.

[2] Angew. Chem. Int. Ed,. 2023, 63, e202313892. DOI:10.1002/anie.202313892

DR. FELIX RIZZUTO

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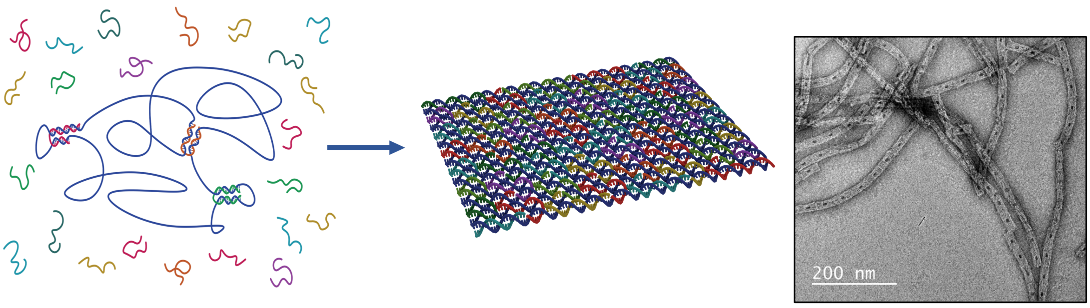
DNA NANOTECHNOLOGY AND ASSEMBLY

Our research looks at new ways of assembling soft materials built from DNA and RNA. We take nucleic acids out of their biological context and use them to construct 'Lego' building blocks and nanorobots for sensing, autonomous devices, and delivery vehicles. Our group is interested in fundamental and applied chemistry, and how we can harness chemical systems to mimic robotic processes, like movement, cargo transport, and actuation. Feel free to email me if you have any questions!

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

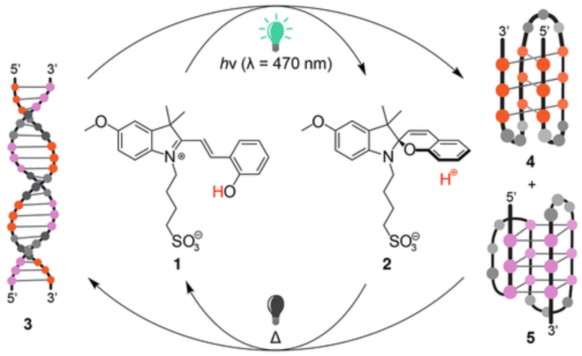
(a) Hierarchical DNA origami assembly

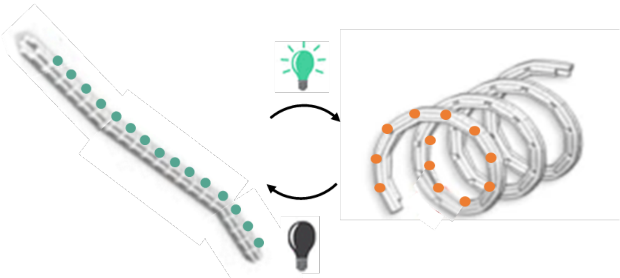


Just like you fold paper into complex shapes like swans and frogs, we can fold DNA into arbitrary geometries, like the bricks shown on the right below. We do this by adding several hundred 'staples' to a large 'scaffold' strand. We are interested in new methods to control this process, and ways in which we can bring these building blocks together to make nanomaterials and DNA polymers. The right is a TEM image where we have built long strings of these structures simply by tuning the sequence of the DNA. We are developing more 'tricks' to connect these bricks together, and to start programming the formation of nanomaterials using only single strands of DNA.

(b) DNA nanomachinery

We are working to make the world's smallest DNA machine that can move, assemble other structures, and deliver cargo, just like a life-sized robot. These 'nanobots' will be able to move molecules between locations, transform their structure, do complex chemistry, and build other nanomachines, with users able to remotely move them whenever and however they want. The problem is that right now we don't have methods to *control* how these machines operate over time – where they go, how fast they get there, and how quickly they perform tasks. This project will develop chemical methods to modulate the movement and transformation of nanomachines, for applications in soft robotics and medicine.

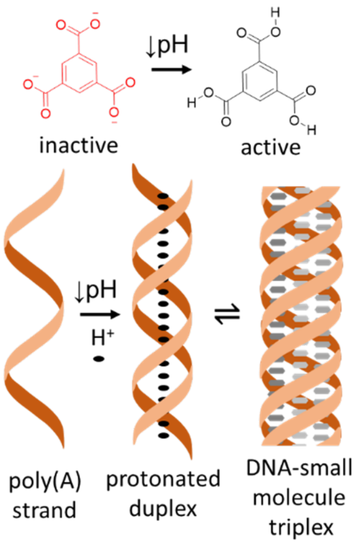




(c) Light-activated and dissipative systems

Light is a powerful stimulus for self-assembly – it can be applied with high spatial and temporal control and does not generate waste, making it highly sustainable. We are interested in using light to control the self-assembly processes of DNA. Recently, we showed that double-stranded DNA could be ripped apart and folded into useful secondary structures using light-activated chemistry (see top right). We have current projects available that explore this process more thoroughly, specifically for catalysis, kinetic modulation, and templated synthesis. This project is in continued collaboration with A/Prof Jon Beves.

(d) Building self-assembled polymers with DNA



Double stranded DNA is an archetype of programmability: the base pairs in DNA mean that we can construct two- and three-dimensional architectures relatively simply. But the range of geometries such structures can take is dictated by the inherent double helix of DNA, limiting the structural and functional diversity of DNA nanomaterials. This project will use small molecules and metal ions to reprogram how DNA self-assembles, producing new structural motifs for nanotechnology applications. We will explore a range of small molecules capable of hydrogen-bonding to common DNA bases and use these structures to build 2 and 3 dimensional constructs that we can image using state-of-the-art microscopy techniques.

Students in my group will also have the opportunity to collaborate with other labs in Chemistry, BABS, and Medicine here at UNSW. All our projects are highly interdisciplinary, spanning chemistry, nanotechnology, biochemistry, medicine, and bioengineering. If anything here sparks interest, do get in touch – we have lots more going on than what I've shown here!

Skills learnt in my group: Biomaterials analysis, non-covalent chemistry, polymer chemistry, self-assembly, stimuli-responsive nanomaterials, microscopy

Read more about our stuff: ***Angew. Chem.,*** 2023*, 62,* e202314458*;* ***JACS***, 2023, 145, 2088; ***Nat. Chem.***, 2021, 13, 843; ***JACS***, 2022, 144, 12272-12279; ***Nat. Mater***., 2020, 19, 1012-1018; ***Chem. Soc. Rev.***, 2020, 49, 4220-4233; ***Nat. Rev. Chem.***, 2019, 3, 204-222.

PROF. TIMOTHY SCHMIDT

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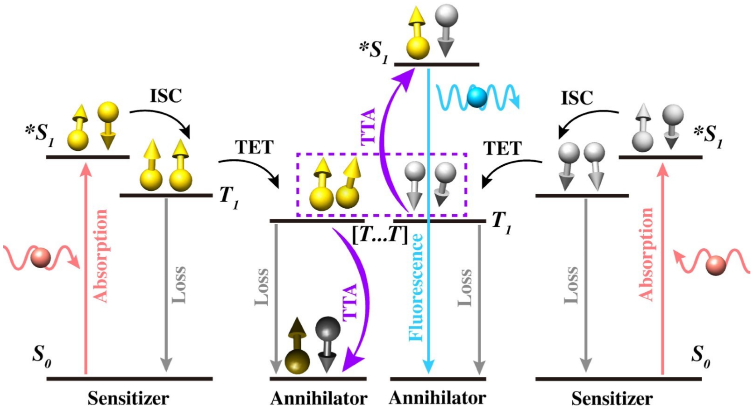
EXCITED MOLECULES

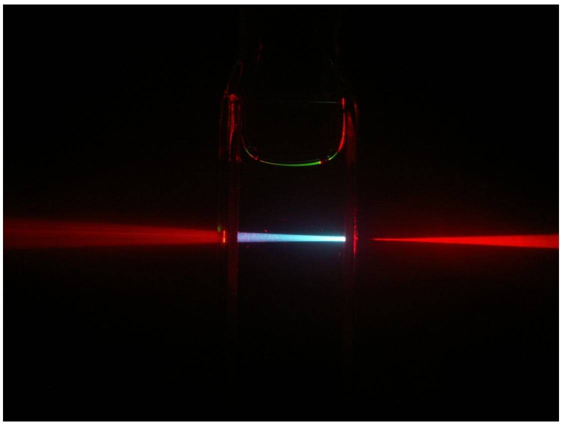
The Schmidt group undertakes research on electronically excited states of molecules. We undertake experiments on molecules in the condensed phase, with applications to renewable energy research, and in the gas phase, with applications in astronomy and astrophysics. We use laser systems with high temporal resolution (10^{-13} s) to watch energy flow in molecule systems, and high spectral resolution (0.07 cm^{-1}) to compare with astronomical observations. We underpin all of our experimental results with appropriate theory and modelling. We have many projects on offer, so come and have a chat!

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

(a) Photochemical Upconversion



What do solar cells, organic light emitting diodes (OLEDs), and hydrogen production have in common? They can all be made more efficient by converting lower-energy excited states into high energy excitations through a process known as photochemical upconversion. By using chromophores to make red light into blue light (or infrared into yellow *etc.*), we can harness more of the solar spectrum, convert dark states in OLEDs into bright states, and increase solar hydrogen production efficiency. To achieve these goals, efficient solid-state upconverters are required.



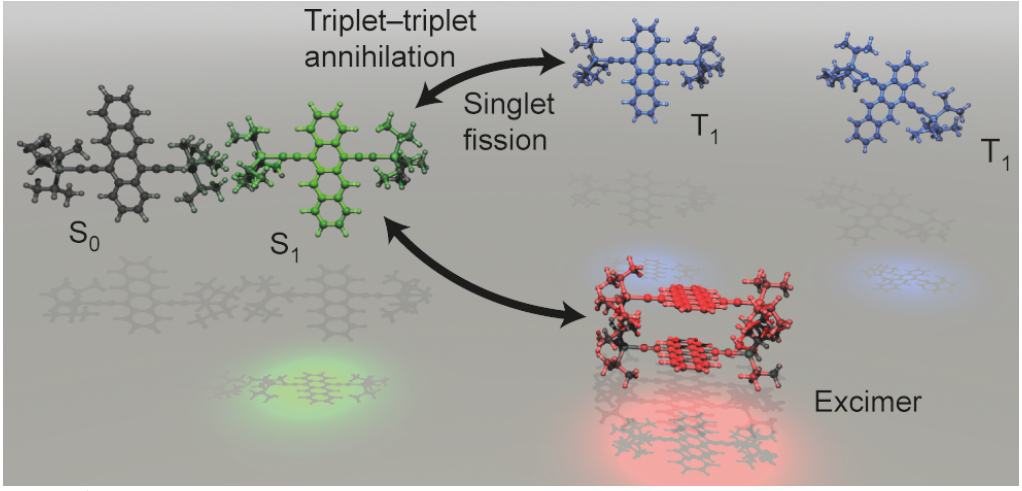
Our group recently showed that by attaching chromophores to a porous scaffold we can achieve efficient solid-state sensitization of upconversion: (https://pubs.acs.org/doi/full/10.1021/acsenergylett.3c01678). In this project we will expand on this work to include new wavelength regions that will benefit solar cells, LEDs, and the photocatalytic production of hydrogen.

What you will do: Organic synthesis, laser spectroscopy, device fabrication, modelling (pick and mix)

(b) Singlet Fission (with Dr Peeks and/or A/Prof. Beves)

UNSW has led the development of silicon photovoltaics (Si-PV). However, Si-PV are fast approaching their maximum theoretical efficiency of 29%. To realise greater efficiencies in Si-PV the fundamental loss mechanism of thermalisation, which accounts for 33% of total losses, needs to be addressed. Thermalisation losses arise because a Si-PV can only use about 1.1 eV of an absorbed photon, no matter its energy. It would be nice if we could split the energy of high energy (>2.2 eV) photons in two!

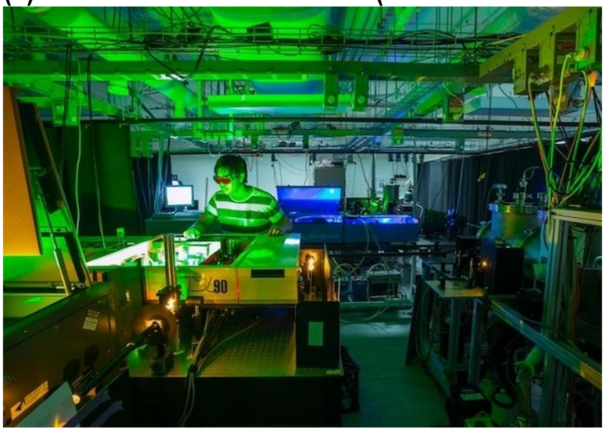
Singlet fission (SF) is such a process. By incorporating a SF capable chromophore with Si-PVs the theoretical efficiency of 29% can be surpassed.



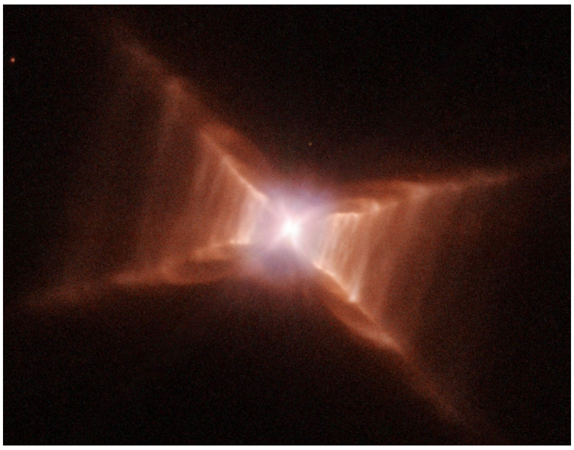
Through the $6M ARENA-funded OMEGA Silicon project (https://www.omegasilicon.solar/) we are developing the next generation of solar cells based on SF. There are multiple potential projects involving SF. If you are interested, please get in contact for more information!

What you will do: Organic synthesis, laser spectroscopy, device fabrication, modelling (pick and mix)

(c) Interstellar Molecules (with Dr Chris Hansen)



The *Molecular Photonics Laboratories* house 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. 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* (DIBs), 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 and radicals (which are the leading candidates for carrying the DIBs), and (hopefully) solve this long-standing problem.



What you will do: Laser spectroscopy, electric discharges, vacuum techniques, quantum chemistry

PROF. NEERAJ SHARMA

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BATTERIES, 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.
- We work with industrial partners to address key challenges.

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

(a) *Really* understanding the chemistry of batteries and making better ones

Lithium-ion batteries are ubiquitous in our daily lives, *e.g.* mobile phones, laptop computers, electric vehicles and energy storage of renewable energy. Alternative battery chemistries are being developed to overcome some of the perceived limitations of lithium-ion batteries, including lithium-sulfur, sodium- and potassium-ion, and all solid-state batteries. Our research group is at the forefront of understanding the chemistry, particularly the structural chemistry, of the materials that make up these devices and the devices themselves. We pride ourselves on using advanced and in-depth analytical methods to understand battery function. With this understanding we can develop even better materials and devices.

A variety of projects are available and these evolve every year. Examples include:

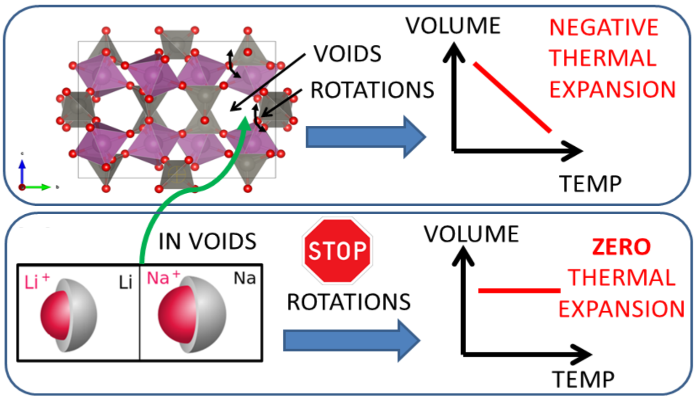
- Synthesis and development of new positive electrode materials for litihium-, sodium- and potassium-ion batteries for more energy dense and longer life batteries – super stable materials.
- Synthesis and development of new solid state electrolyte materials for all solid-state batteries.
- Use of renewable and/or sustainable sources as materials for batteries. For example, working with waste such as coffee grinds or food acids to make electrodes for lithium-ion batteries.
- Diagnosing degradation in batteries using advanced characterisation techniques, such as synchrotron or neutron diffraction or micro X-ray computed tomography.
- Investigating alternative and sustainable processing techniques for electrodes and electrolytes.
- Scaling up in-house developed electrode and electrolyte materials.

(b) Innovative recycling of batteries and battery materials

As the uptake of lithium-ion batteries dramatically increases, a challenge that will face the world both now and in the future is ***what to do with end-of-life batteries?*** The Sharma group is taking an active role in this by developing chemical processing techniques that can allow the effective and efficient recycling of battery materials and their re-use in other applications or back into batteries. We use our characterisation know-how to develop routes for recycling and new concepts in this space, often working with industrial partners or opening up batteries in our dedicated argon glovebox. We aspire to have solutions available as lithium-ion battery recycling becomes essential.

(c) 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.



(d) Industrial collaborations

Projects with industrial partners

A variety of industrial-focused projects are being undertaken in the Sharma group and as an honours student you can undertake such a project. An example, Orica is looking to electrify its fleet of vehicles and is interested in understanding the interplay between dangerous goods, including explosives and explosive precursors, and lithium-ion batteries. We have a number of projects trying to understand how such materials and explosions ***impact*** lithium-ion batteries and the materials that make up lithium-ion batteries.

Projects with ANSTO minerals: Ore to materials

ANSTO minerals works with numerous industrial partners to unlock value from Australian minerals, via chemical processing, purification and in some cases recycling. The Sharma group works with collaborators at ANSTO on the chemistry of such processes - to investigate methods to improve processes using our characterisation know-how. As an honours student a variety of projects are available including but not limited to battery materials.

(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.

SCIENTIA PROF. MARTINA STENZEL

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NANOPARTICLES AND NANOPLASTIC- opportunities and challenges with polymers

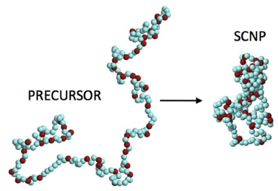
We are a polymer group that is interested in plastic on the nanoscale!

We have a big research program on nanomedicine: The delivery of drugs can be improved by packaging the drug into nanoparticles. Nanoparticles for drug delivery typically have 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.

Although polymer nanoparticles can help with treating diseases, micro-and nanoplastics found in the environment can potentially be dangerous to living beings, but nobody really knows. We assist the discussion by understanding how nanoplastics can absorb pollutants and cause toxic effects.

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

Nanomedicine



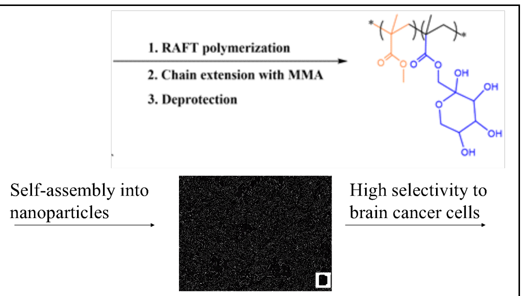
From polymer chain to single chain nanoparticle

(a) Making really small polymer nanoparticles for the delivery of drugs

Most nanoparticles used for drug delivery described in the literature are larger than 20 nm. However, there are various reasons to create smaller nanoparticles, such as improved circulation time in the bloodstream and better diffusion into tumor tissue. To achieve this, we prepare polymers with attached drugs in different amounts and sequences. These polymers are then collapsed into single-chain nanoparticles (SCNP), which are typically under 5 nm in size. This project requires students with interest in organic synthesis.

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

Carbohydrates are involved in a number of biological communication events as they carry sugar-specific receptors. This specific sugar-receptor interaction can be used to deliver nanoparticles specifically to receptor-expressing cells, which can result in improved biodistribution. Synthetic polysaccharides, coined glycopolymers, have been shown to be superior to single sugars as they can bind simultaneously to several receptors. In this project, we would like to develop glycopolymers for the delivery of drugs to brain



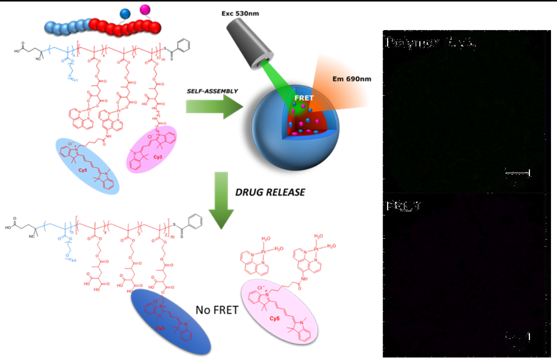
Synthesis of glycopolymers and their self-assembly into nanoparticles cancer. We will entrap anti-cancer drugs that are specifically developed in the school of medicine against brain cancer. If time permits, the drug carrier will be tested on brain cancer cell lines.

(c) Learning more about the structure – solid state NMR

In collaboration with the NMR unit, we will learn more about the interior of polymer nanoparticles and their payload. This project is for student who would like to learn high-end NMR spectroscopy

(d) Where is the drug? – Fluorescence studies to monitor drug release

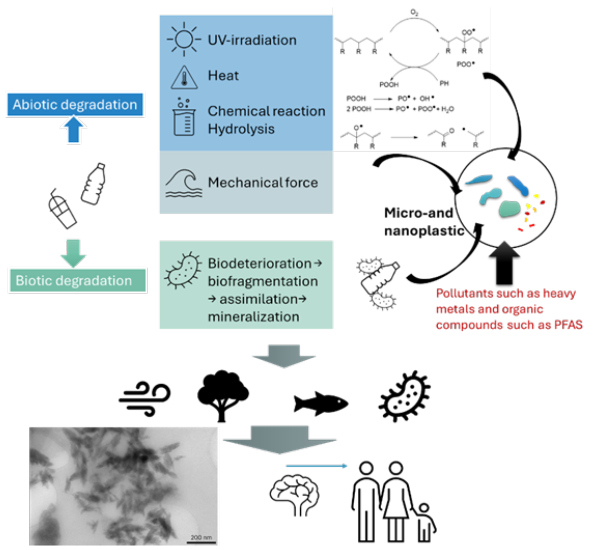
Key to the success of drug delivery with nanoparticles is the entrapment of the drug inside the nanoparticle, only to be released when the nanoparticle is inside the targeted cell. One way of monitoring the release is to monitor the fluorescence of the drug carrier and that of the drug. If the drug is entrapped inside the carrier, Förster resonance energy transfer (FRET) occurs. If the drug is released from the nanoparticle, fluorescence changes. FRET can be used to monitor the drug release in live cells, which can help us make a decision on how to improve our drug delivery system.



Analysis of drug release inside the cell using fluorescent studies

Nanoplastic

Everyone has heard of microplastics, but the term nanoplastic (below 1000 nm) is only now entering the public consciousness. Recent articles showed that we have large amounts of nanoplastics in our oceans—an amount that far exceeds microplastics. Furthermore, plastic has been found in the brain (see picture), and closer inspection revealed it to be nanoplastic. We do not yet know how dangerous plastic truly is to our health, but initial reports, often using engineered micro- or nanoplastic beads, suggest it could be harmful.



Pathways of plastic degradation. The inserted TEM shows the nanoplastic pieces found in the brain

In this study we will look at accelerated ageing of plastics, the formation of nanoplastic and the ability of nanoplastic to absorb environmental pollutants such as metal ions and PFAS. We can potentially also study toxicity using some immune cells as part of your honours project.

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MATERIALS CHEMISTRY AT THE NANOSCALE

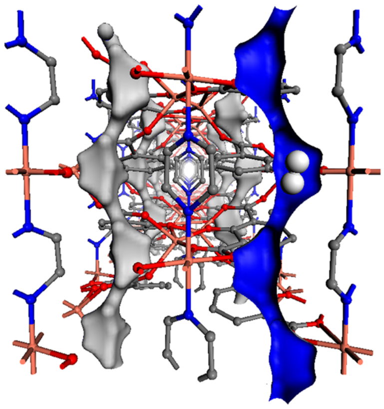
My group focuses on making and understanding new materials that are often focused on some of the major challenges facing us today: energy, water and sustainability. We make use of a range of techniques that include X-ray and neutron scattering in truly multi-disciplinary projects. Key to these studies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

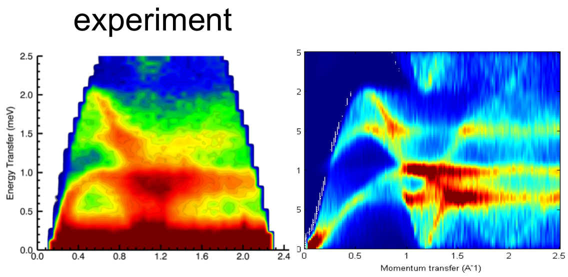
Sorting and storing molecules - how to select for one molecule over another



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.

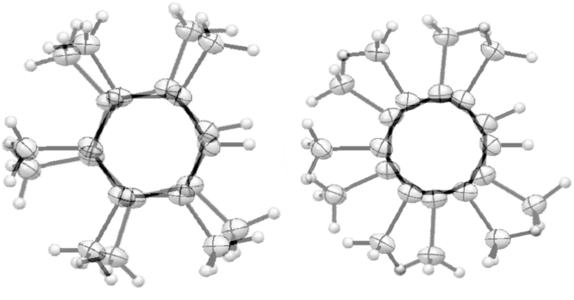
Quantum phenomena in magnetic materials

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.



(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.



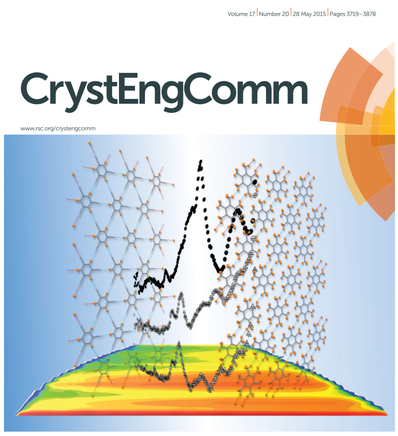
(a) crystalline phase (b) plas1c phase

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.[1] 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.

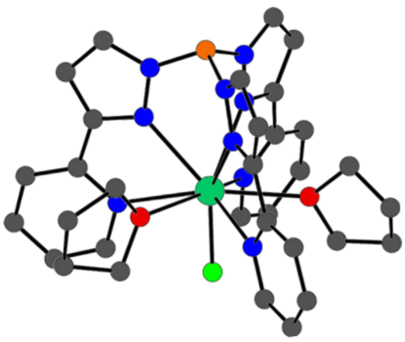
Skills you will learn:

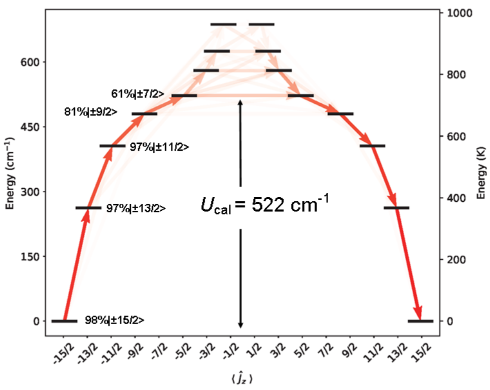
- Manipulation of air- and moisture-sensitive compounds
- Organic and Inorganic synthetic chemistry
- Structure elucidation – NMR spectroscopy (^{1}H, ^{13}C), IR spectroscopy, SQUID magnetometry and XRD (Yeap, we grow crystals)!

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

(a) Scorpionate Ligands in Lanthanide SIMs

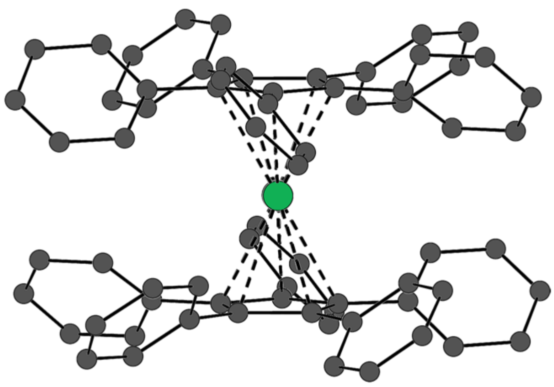
Ongoing research into Single-Ion Magnets (SIMs) is of great interest due to their potential applications in molecular storage devices and as Qbits in quantum computing. SIMs retain their orientation of magnetisation in the absence of a magnetic field due to having a barrier to said reorientation. Record SIM barriers utilise cyclopentadienyl ligands, these have several drawbacks and as such in the Sulway group one aspect that we explore are isolobal systems such as scorpionate ligands.[2]

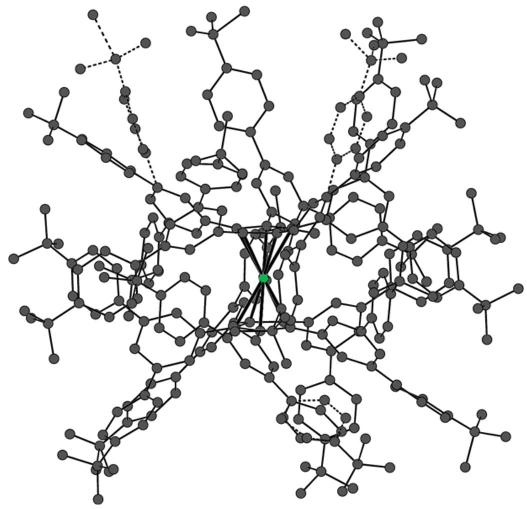




(b) Exploring Alternate Cyclopentadienyl Ligands in SIMs

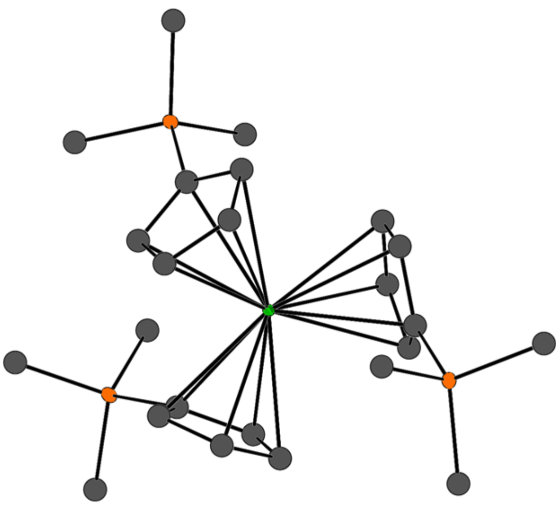
As described in project (a) the current record barriers in SIMs utilise the cyclopentadienyl moiety, we also look into these systems focusing upon bulkier ligands. These systems are great if you want to combine some inorganic and organic synthesis.

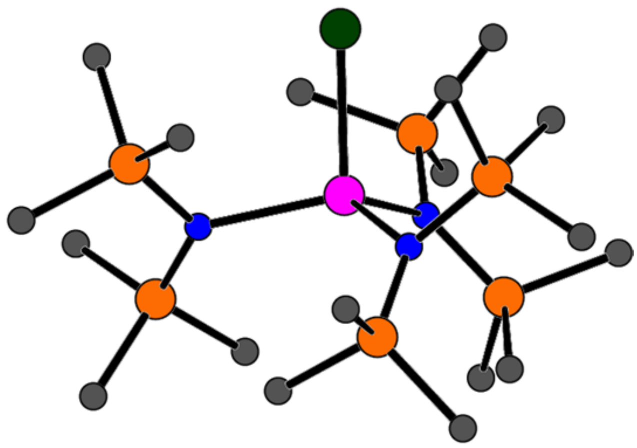




(c) Equatorial Ligands in Prolate Lanthanide Ions

How about something a little different? SIM research often focusses on axial systems, equatorial systems are very rarely studied and not very well understood. We work on trying to expand the understand in this emerging area by looking into the "neglected" lanthanide ions.





(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. (a) Goodwin, C. A. P., Dalton Trans., 2020, 49, 14320-37, (b) Woodruff, D. N.; Winpenny, R. E. P.; Layfield, R. A., Chem. Rev., 2013, 113, 5110-48, (c) Rinehart, J. D.; Long, J. R., 2011, 2, 2078-85.
2. Thomas, J. R.; Sulway, S. A., RSC Adv., 2021, 11, 16158-60.

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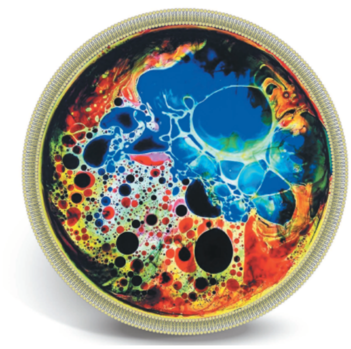
RNA CHEMISTRY, ORIGIN OF LIFE AND NANOMEDICINE

- **RNA Chemistry** with focus on understanding how RNA interacts with peptides other molecules and how these interactions can be applied in RNA science and therapeutics
- **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 **catalysis** and **medical research**
- **Synthesis** of novel **peptides** for **nanomedicine**, including drug delivery and tissue engineering

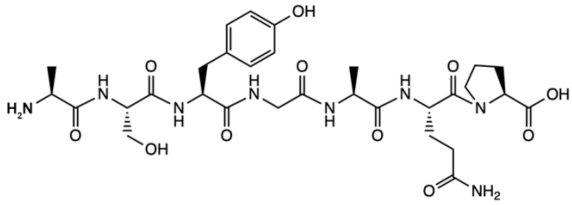
It would be great to work with Honours students on the following projects:

(a) Peptide-RNA interactions – solving pressing problems in prebiotic chemistry and medicine *(Potential for collaborations with Dr Albert Fahrenbach & A/Prof. Anna Wang School of Chemistry).*

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:

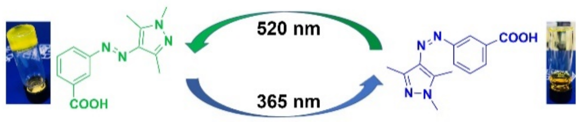


Did the cell start of as a collection of peptide-RNA "droplets"? And is this how the cell is really organised? (from E. Dolgin, Nature 2018, 555, 300.



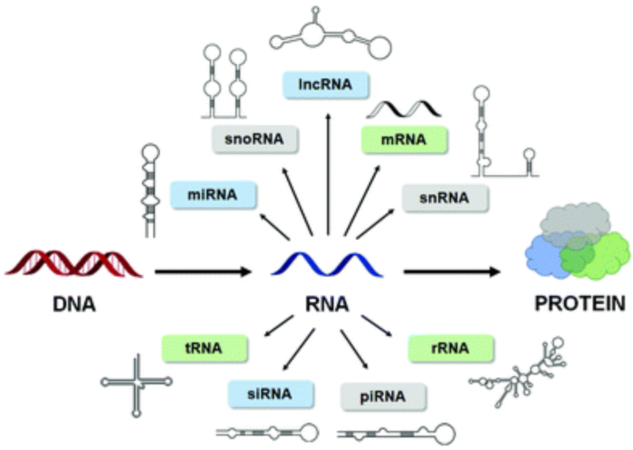
(b) Novel switchable and hybrid peptide-based materials for catalysis and 3D cell cultures *(Potential for collaborations Prof. Jonathon Beves, A/Prof. T. Vinh Nguyen and Prof. Kris Kilian, School of Chemistry).*

Self-assembled peptide gels have already been proven to be useful as 3D material for growing living cells, even neurons.[4] We have extended this work to include the formation of gels that can changed through a photo-switch,[5] or mixing with a biological material such as collagen. In more recent work we also been able to demonstrate that self-assembled gels can be used as a scaffold for catalysis in chemical synthesis. Projects involving developing novel photo-switchable and hybrids gels applications in cell biology and catalysis are available for those with interest in medicinal chemistry, nanomedicine, supramolecular and synthetic chemistry.



(c) Novel RNA therapeutics *(Potential for collaborations with Dr Chantelle Ahlenstiel, Kirby Institute UNSW, Dr. Daniel Ferandez Ruiz, School of Biomedical Science and Prof. Maria Kavallaris, Children's Cancer Institute Australia).*

Ribonucleic acid (RNA) is now recognised to play a much more important role in biology than previously thought. It is not merely a "messenger" (mRNA) but has many other functions in the cell. From a chemist's point of view the structural diversity of these different types of RNA molecules is fascinating (see Figure from a recent review by the Disney group,[6]). Many of these RNA molecules play a crucial role in diseases. Inhibiting or regulating RNA function through the application of small molecules, peptides or specially designed RNA molecules such as small interfering RNA (siRNA) therefore represents a powerful strategy to develop new and better therapeutics for cancer, infectious diseases (including HIV and COVID-19) and various disorders that have genetic origin or relate to gene expression misregulation. Projects, including with our collaborators, involve developing novel peptide binders for disease-causing RNA motifs, synthesis of novel siRNA molecules and siRNA-ligand conjugates 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. Adam D. Martin, Sook Wern Chua, Carol G. Au, Holly Stefen, Magdalena Przybyla, Yijun Lin, Josefine Bertz, Pall Thordarson, Thomas Fath, Yazi D. Ke and Lars M. Ittner, Peptide nanofiber substrates for long-term culturing of primary neurons, *ACS Applied Materials & Interfaces*, **2018**, 10, 25217-25134.
5. Fayaz Ali Larik, Lucy L. Fillbrook, Sandra S. Nurttila, Adam D. Martin, Rhiannon P. Kuchel, Karrar Al Taief, Mohan Bhadbhade, Jonathon E. Beves* and Pall Thordarson*, Ultra-Low Molecular Weight Photoswitchable Hydrogelators, *Angewandte Chemie International Edition*, **2021**, *60*, 6764-6770.
6. S. M. Meyer, C. C. Williams, Y. Akahori, T. Tanaka, H. Aikawa, Y. Tong, J. L. Childs-Disney, M. D. Disney, Small molecule recognition of disease-relevant RNA structure, *Chem. Soc. Rev.*, **2020**, 49, 71767-7199.

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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.

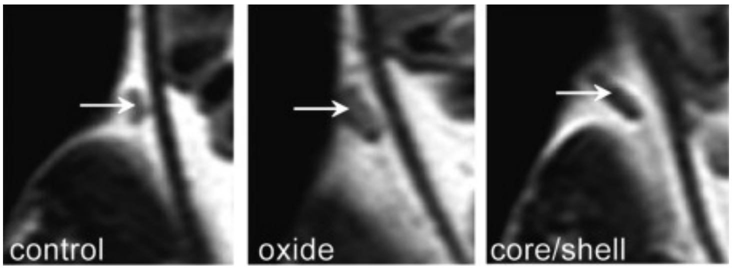
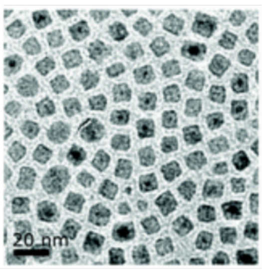


Figure 1: MRI images from iron nanoparticles injected into a mouse to enhance the contrast of a tumour.

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.



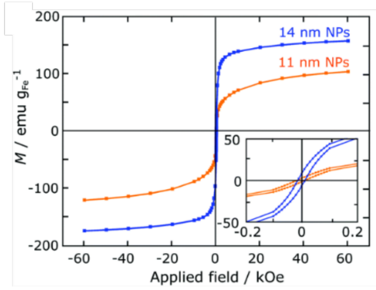


Figure 2: Transmission electron microscopy images of iron nanocubes and their magnetic properties for use in MPI.[1]

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).

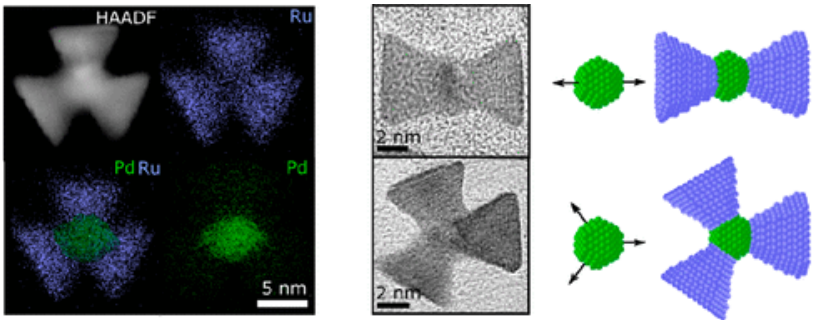


Figure 1: Energy dispersive X-ray spectroscopy elemental mapping of Pd-Ru branched nanoparticles and TEM images of individual nanoparticles. Models show the controlled direction of growth of Ru from Pd seed.

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]

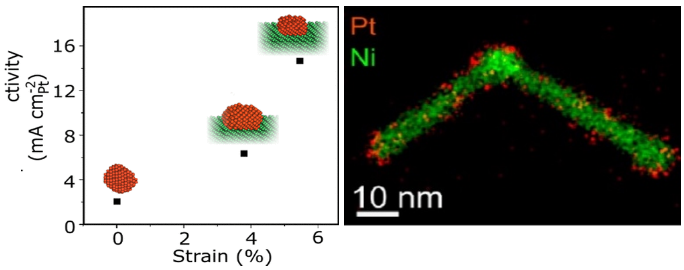


Figure 1: Relationship between strain and HER activity and elemental map of a Pt on Ni nanoparticle.[2]

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

- How did the first cells on Earth form? One of our main interests is in lipid bilayers (Fig 1), which encase our cells but are also used for drug delivery.
- One of our other main interests is in how matter interacts with light, which we study with holographic imaging and light scattering calculations.
- We tackle problems at the nexus of chemistry, physics, biology, and materials science.
- Our group has students from many backgrounds – interdisciplinary problems require multidisciplinary teams of problem solvers.
- Students typically work with biomaterials like lipids, RNA, and gels, and do microscopy, optics, image analysis, data analysis and calculations with Python.
- We have ongoing international collaborations, including with industry.

It would be great to work with students on the project topics (a) – (e):

(a) Building an artificial cell life cycle

Being able to create a self-perpetuating artificial cell (Fig 2) reflects an unprecedented understanding of lipid bilayers and living systems, and is an overarching goal of our group's. Outstanding questions include:

- How can we control the fusion of lipid compartments by modulating their composition?
- How do we get these compartments to grow and divide?
- How do different populations of lipid vesicles/liposomes compete with each other?
- How does crowding inside cells and artificial cells affect diffusion rates and membrane shape changes?

The answers to these questions are important for understanding how evolution could have been kickstarted at the origins of life (Fig 2). They will also reveal fundamental membrane biophysics, with implications in drug delivery processes.

Students will learn lipid manipulation techniques, lipid vesicle/liposome processing techniques, fluorescence spectrophotometry, microscopy, and biophysics assays.

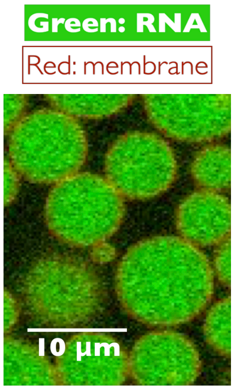


Fig. 1 Liposomes containing RNA

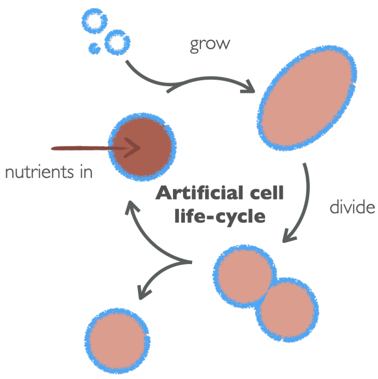


Fig. 2 A dynamic growing system

Key papers include ones on protocell survival (Small, 2025), endocytosis in model protocells (PNAS, 2023), model protocell fusion (Small Methods, 2023), and protocell self-assembly (ACS Nano, 2020).

(b) Characterising liquid-liquid phase separation with holographic microscopy

Liquid-liquid phase separation (LLPS) is a supramolecular phenomenon whereby macromolecules interact and condense into one liquid phase (dispersed in another). RNA and peptides, for example, undergo LLPS in cells. LLPS also occurs in secondary organic aerosols.

LLPS is also a first step in many diseases, including Alzheimer's, because LLPS droplets are only metastable. How do such droplets transition to a disease state?

The student will develop a mechanistic understanding of LLPS, which involves the characterisation of LLPS at a single-droplet level. This project will use holographic microscopy to characterise LLPS systems, revealing how their size density evolves over time. Holographic imaging of colloidal particles trapped in LLPS droplets will reveal the viscosity of the internal droplet environment. Recent papers include "Using holographic microscopy to measure the effect of confinement on crowding agents in lipid vesicles" (ChemBioChem, 2023)

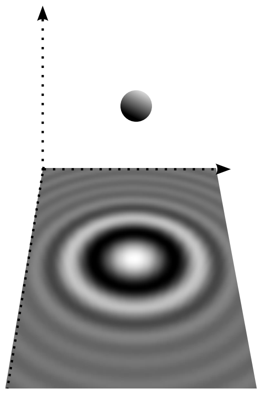


Fig. 3 Hologram of droplet

(c) Designing particles with novel optical properties for printing, cosmetics, and electronics

This project involves using light scattering software to help design particles with intriguing optical properties e.g. transparency in the visible and high scattering in the UV. These novel particles could increase the efficiency of inks, sunscreens, electronics, and more. No background in Python needed, we'll teach you what you need to know. Recent papers include "In-line holographic microscopy with model-based analysis" (Nature Reviews Methods Primers, 2022).

(d) Measuring cellular forces for improved material design (in collaboration with A/Prof. Kris Kilian)

The mechanical environment of cells often determines their fate. To design better tissue engineering scaffolds and materials, we must first measure how cells push and pull on their environments. We propose using holographic imaging (Fig. 4) to solve this problem.

The student will pioneer and then use holographic traction force microscopy to investigate focal adhesion and traction stress propagation from adipose derived stem cells (ADSCs) adherent to the surface. Relationships between cell generated traction and differentiation to adipocyte, chondrocyte, and osteoblast lineages will guide the design of materials for tissue engineering and regenerative medicine

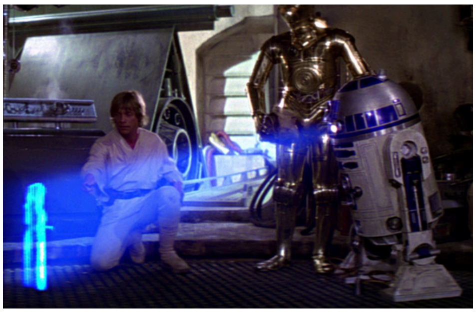
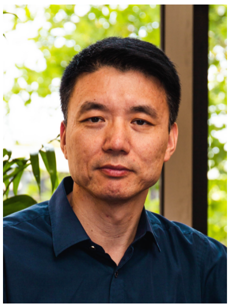


Fig. 4 "Holographic imaging" in the movies

(e) A project of your choosing (and imagination)

There are many more possible projects in our group pertaining to artificial cells, origins of life, soft matter, microscopy, and more – speak to Anna to see what's possible, we collaborate with many groups in the School.



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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, fuel cells, ammonia synthesis, gas sensors, and proton batteries.

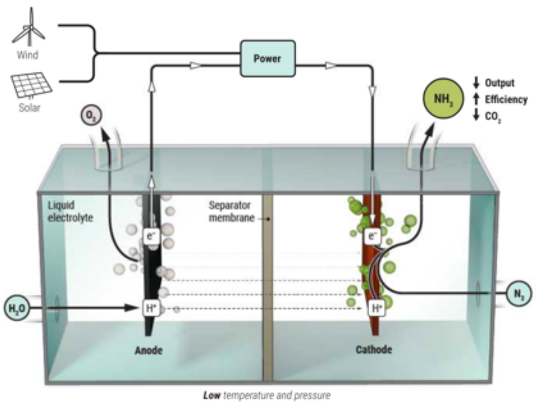
It would be great to work with Honours students on the following projects:

(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) Electrocatalytic Synthesis of Ammonia from Renewable Hydrogen and Atmospheric Nitrogen

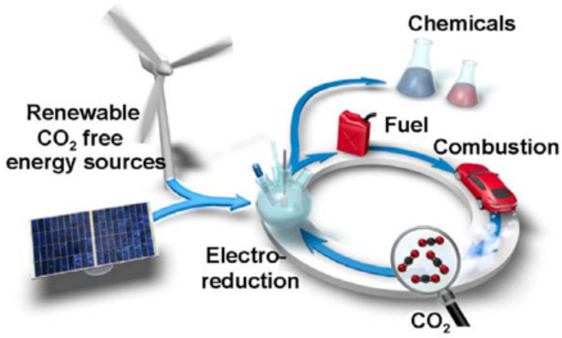
Ammonia (NH_3) is one of the most important and widely produced chemicals worldwide for fertiliser production and is also a promising liquid hydrogen carrier to be used as a carbon-free fuel. N_2 has a very strong triple bond and is extremely inert. Currently, the synthesis of NH3 is still dominated by the high-temperature and high-pressure Haber-Bosch process developed in the early 1900s, which is one of the top largest chemical processes in terms of energy consumption and greenhouse gas emissions.



This project aims to develop a sustainable electrochemical nitrogen reduction reaction (NRR) at ambient conditions powered by renewable energy sources. Our group has recently made breakthrough in developing metal-organic framework (MOF) based catalyts for NRR. In this project, the student will have opportunity to work on these advanced electrocatalysts and evaluated their performance for ammonia synthesis using renewable electricity, hydrogen and atmospheric nitrogen.

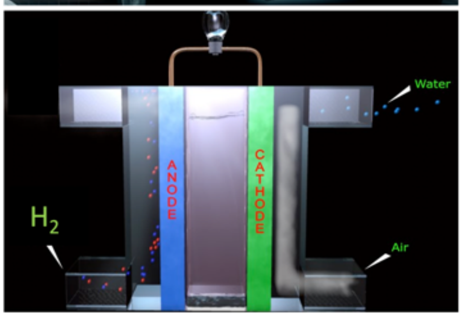
(c). Conversion of CO_2 to Fuels with Renewable Electricity and Earth Abundant Catalysts

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.



(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, and are particularly attractive for larger (e.g. SUV) and longer-range vehicles. 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.

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ORGANIC SYNTHESIS FOR MEDICINAL CHEMISTRY AND MATERIALS

Synthetic organic chemistry is the discipline responsible for building the molecules that have transformed science, technology, and everyday life and the group aims to make inroads into all of these areas. There are many different topics that an Honours student can contribute to the group's research. These can be targeted to match your interests. Whether it is medicinal chemistry, materials or just exploring what can be achieved with organic chemistry, then we have something for you.

Please note that these projects can only be hosted at the Canberra campus of UNSW

a) **Novel bioisosteres for medicinal chemistry**

To build new medicines, agrichemicals, and advanced materials, synthetic chemists combine building blocks with defined shape and size. The largest proportion of available building blocks are flat (achiral) aromatic compounds, which are readily available, well-studied and undergo a wide range of useful reactions. In a three-dimensional world, these flat building blocks severely constrain chemists' ability to invent new life-changing molecules and materials. Access to building blocks that possess all the benefits of aromatic compounds, but that also incorporate three-dimensional shape (and chirality) is a pressing unmet need. The development of new molecular systems typically involves altering the groups attached to the flat aromatic core of privileged molecular fragments (*peripheral substitution*). However, the use of *internal substitution* to tune structural, electronic and chiral properties of molecules is unexplored (Fig 1.). This project will explore both the chemical reactivity of these types of compounds as well as their potenital to be incorporated into drug molecules as isosteres of naphthalene.

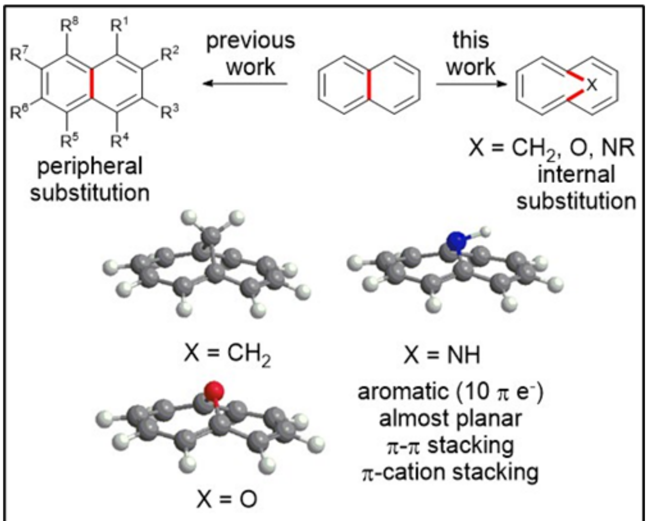
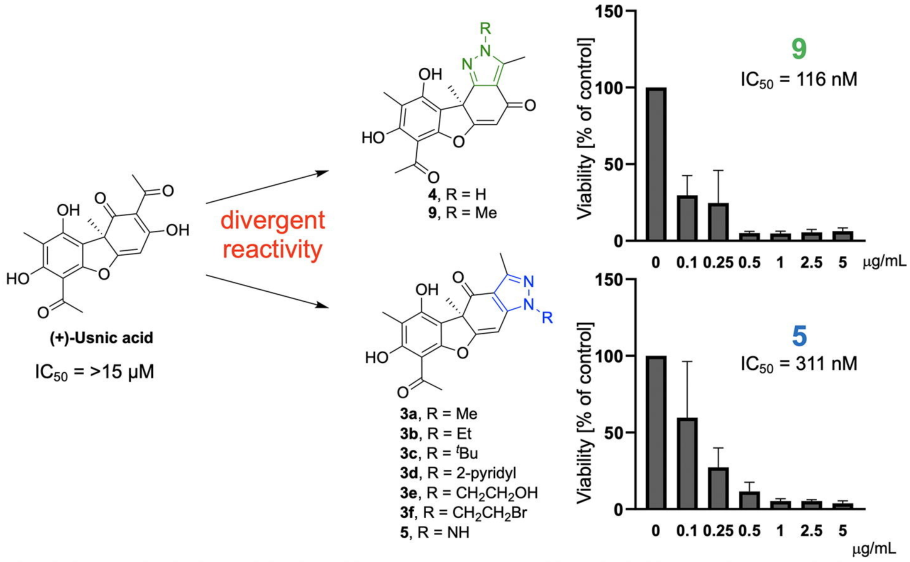


Fig. 1.Overview of internal arene substitution.

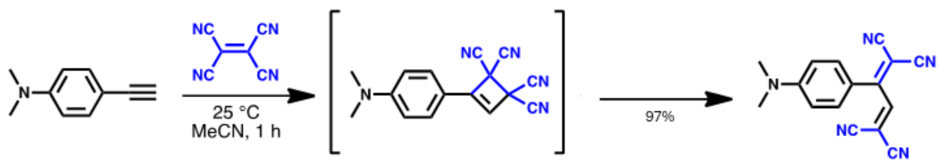
b) **Utilising natural products as starting materials for drug development**



Natural products are small molecules produced by plants, microbes, and marine organisms and are widely used as starting points for drug development. This is because their complex and diverse chemical structures often display intrinsic bioactivity, making them valuable “lead compounds” for therapeutic discovery. Many successful drugs, including antibiotics, anticancer agents, and immunosuppressants, are either natural products or derivatives thereof, illustrating how nature-inspired scaffolds continue to guide modern pharmaceutical innovation. However, they can often be classified as poor drugs due to their poor stability, selective or bioavailability. This project will utilise readily available natural product usnic acid as a starting point to generate novel molecules designed to target cancer cells.

c) **Small-molecule chromophores**

Small-molecule chromophores are valuable tools across chemistry, biology, and materials science because of their ability to absorb and emit light in a predictable manner. This optical responsiveness enables their use as fluorescent probes for imaging and sensing or in modern applications such as waveguides. We have identified a simple synthetic route to easily generate highly coloured small-molecules in a single step. This project will explore this reaction further as well as analyse the optical properties of the products generated.



Frequently asked questions

Do you have more questions?

- See the CHEM4516 and/or CHEM4508 handbook
- Please email the School of Chemistry Honours coordinator. Email: chemhonoursadmin@unsw.edu.au

Who can apply?

- We welcome all Science graduates from all over the world to apply
- See “Honours eligibility” for specific details

Do you have to enrol in Honours full time?

- No! You need to complete 48 UoC in total
- CHEM4516 is to complete the course full-time across one year. Students are enrolled in the course over three terms (3 x 16 UoC).
- CHEM4508 is to complete the course on a part-time basis. Students are enrolled in the course over six terms (6 x 8 UoC)

What are the intake periods?

- Term 1, Term 2 or Term 3

When does Honours commence?

- Honours commences on Monday of Week 1 of each Term

Project/supervisor allocation

- The school allocates a supervisor and project to you. You are required to nominate a minimum of three supervisors in order of preference
- It is expected that you meet and discuss possible projects with potential supervisors before nominating them on your application
- 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(s)

Is it possible to do a joint project with other Schools at UNSW?

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

Is it possible to do Honours at UNSW Canberra?

- UNSW Canberra School of Science also carry out experimental chemistry research that may be of interest
- Projects may be undertaken directly with the School, or in collaboration with UNSW School of Chemistry researchers
- Please contact the Honours coordinator for more details