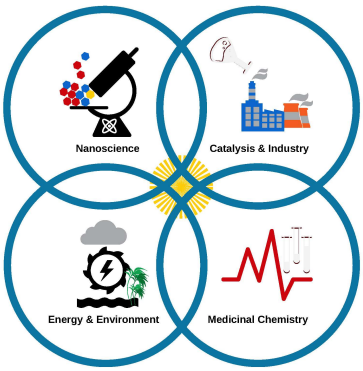
UNSW AUSTRALIA

Never Stand Still | Science | School of Chemistry

CHEM2999 & CHEM3998 Research Projects in Chemistry 2023

WELCOME

The School of Chemistry at UNSW is one of the leading centres of chemistry research in Australia. Composed of over 30 well-funded **research teams**, we are located in the following buildings on lower campus: Dalton (F12), Chemical Sciences Building (F10NA and F10), the Hilmer Building (E10) and the Science and Engineering Building (E8). The School has state of the art research facilities that enable research spanning the entire breadth of chemistry. The UNSW Mark Wainwright Analytical Centre (MWAC) is co-located adjacent to the School of Chemistry (F10NA) and provides major research facilities that are unsurpassed internationally.



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

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

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

The School of Chemistry at UNSW has strong links to Australia's professional body for chemists, the Royal Australian Chemical Institute **(RACI)** and the International Union of Pure and Applied Chemistry **(IUPAC)**. It also has close ties with the American Chemical Society **(ACS).** Several research team leaders hold senior positions in the RACI, and the NSW state branch is located in the School. Professor Sir Fraser Stoddart (2016 Nobel Laureate) has also commenced research activities within the School.

The School welcomes applicants for Chem2999/Chem3998 undergraduate courses. Further we welcome applications for Honours from students throughout the world, acknowledging that the Honours year is an outstanding research experience. We are confident that the wide range of research undertaken in the School provides applicants with a rewarding Chem2999/Chem3998 program and Honours year.

Professor Scott Kable (Head of School)

Dr. Laura McKemmish (CHEM2999 and First Year Research Coordinator)

Dr Neeraj Sharma (Chemistry Honours & CHEM3998 Coordinator)

OVERVIEW OF UNDERGRADUATE RESEARCH PROGRAMS CHEM2999 & CHEM3998

This booklet provides details of the CHEM2999 and CHEM3998 courses, in which students undertake an authentic short research project under the direction of a Chemistry academic member of staff taking advantage of UNSW's world-class researchers and research facilities. Student engage directly with academics and their research group, becoming involved with the group's regular activities such as group meetings, while learning important research and transferable graduate skills prized throughout academia, industry and business.

Both courses require a WAM of at least 65 and are offered in all three terms and in summer. Enrolment occurs every term.

CHEM2999 – Special Project in Chemistry

This course is most suitable for students in their second year with only first-year Chemistry background. It provides an early introduction to the university research environment. A particular focus of this course is communicating the complex research topic to a scientifically-literate non-expert audience.

CHEM3998 – Advanced Special Project in Chemistry

This course provides a more sophisticated introduction to the university research environment than CHEM2999 with a more complex project that utilises the skills and knowledge obtained by students in their early undergraduate degree. Students thus need to have completed at least 18 UoC of second year subjects OR 36 UoC of Level II Science or Engineering Courses to take this course.

These courses are designed to pave the way into Honours. However, you can most certainly undertake Honours without these courses.

For summer term research, students will need to find an appropriate academic who will be available for this period.

For each course a 1 hr fortnightly session is allocated but will be used as required for training, skills development, reflection and cohort building.

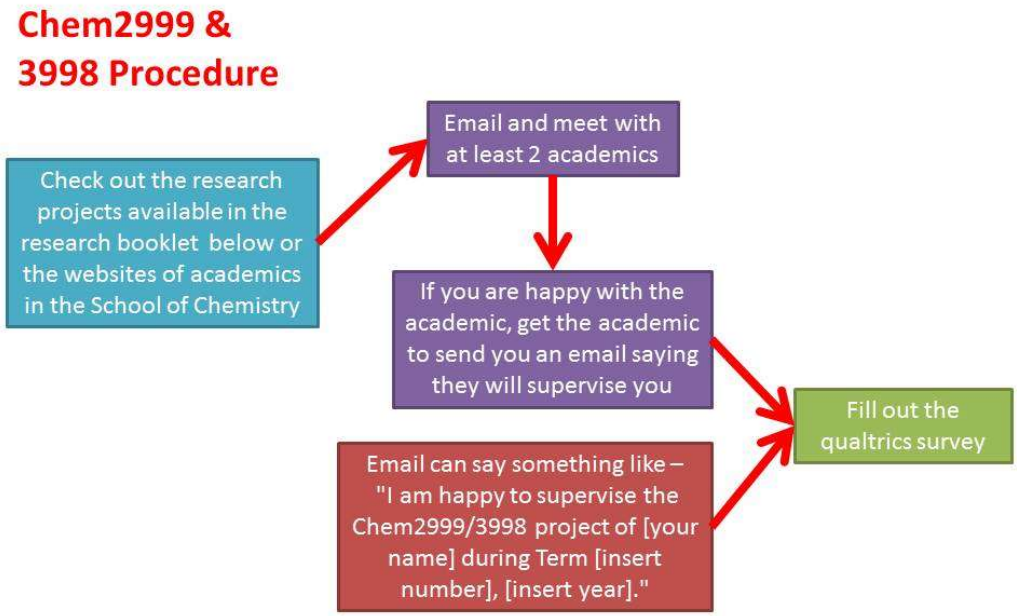
THE ENROLMENT PROCEDURE

Students can enrol in CHEM2999 and CHEM3998 for any term in the UNSW3+ model. The enrolment will occur prior to each term commencing (typically during the exam period the preceding term).

Please note, enrolment into these courses is not available directly through my.unsw. Students need to talk to academics, obtain approval and submit the form (https://unsw.au1.qualtrics.com/jfe/form/SV_0qWMk0RH8FFRppr). **Students will be enrolled by the School of Chemistry at during the exam period in preceding term or before the commencement of the term (in the case of T1) If students require confirmation or enrolment earlier please contact the Coordinators.**

A WAM of 65 is typically required to undertake these courses. Please note, a WAM check will be performed before enrolment is approved.

The procedure:



The form can be found:
https://unsw.au1.qualtrics.com/jfe/form/SV_0qWMk0RH8FFRppr

For further details, please touch base with the Chem2999 and Chem3998 Coordinators Dr. Laura McKemmish (l.mckemmish@unsw.edu.au) or Dr. Neeraj Sharma (neeraj.sharma@unsw.edu.au).

Typical deadlines for Chem2999 and Chem3998

Term 1

Online form submitted by Wednesday Week 10 Term 3, the year preceding

Enrolments will occur on during the exam weeks of Term 3 or after the release of results depending on the WAM check

Term 2

Online form submitted by Wednesday Week 10 Term 1

Enrolments will occur on during the exam weeks of Term 1 or after the release of results depending on the WAM check

Term 3

Online form submitted by Wednesday Week 10 Term 2

Enrolments will occur on during the exam weeks of Term 2 or after the release of results depending on the WAM check

Summer Term

Online form submitted by Wednesday Week 10 Term 3

Enrolments will occur on during the exam weeks of Term 3 or after the release of results depending on the WAM check

ASSESSMENT

Both courses are pass/fail.

Both courses require attendance to an fortnightly meet-up. This is a key component of the revised courses. It will enable students to build stronger supportive peer networks, discuss research careers and culture. It will provide an opportunity to practice short informal presentations to a non-specialist audience. Most importantly, these meetings will facilitate students in developing a high level of meta-cognition of the technical and transferable skills they are developing during their research placement, essential when applying for PhD positions and jobs in the future.

Both CHEM2999 and CHEM3998 requires the submission of a scanned copy of the laboratory notebook (or equivalent) and an excel spreadsheet (summarising activity) in Week 5 and Week 10 of each Term. Submission of a final report is required in Week 11 of each Term. Feedback is provided the week after each submission.

The two courses will be distinguished by the standard of research expertise that students must demonstrate to successfully pass this course, along with a different focus area in the final report: CHEM2999 students focus on contextualising their research while CHEM3998 students focus on identifying fruitful future directions of their research.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CHEM2999 & CHEM3998 SUPERVISORS

DR. GRAHAM BALL

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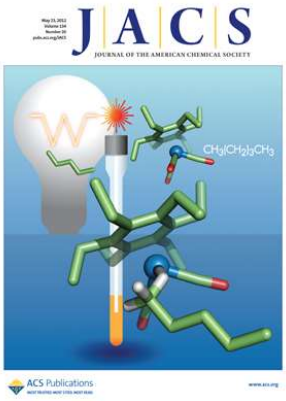
NMR SPECTROSCOPY AND COMPUTATIONAL CHEMISTRY: APPLICATIONS TO ORGANOMETALLIC AND BIOLOGICAL CHEMISTRY

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

Our experimental work is complemented and enriched by using computational techniques. We model small chemical systems with *ab initio* and DFT methods and 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

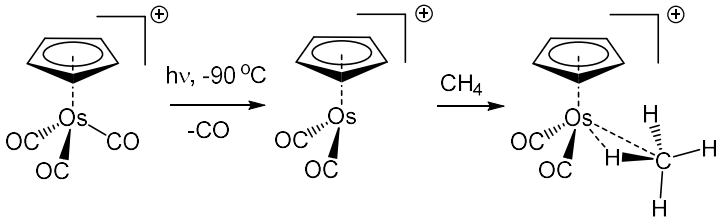


We use photochemistry in combination with *in situ* NMR at low temperatures to study molecules that have fleeting existence at room temperature. With this strategy, we have observed several types of alkane complex[1,2,3] including the *JACS* cover opposite[1] and even complexes where xenon acts as a ligand.[4] Alkanes contain no lone pairs for binding to the metal centre. Instead, they bind using the electrons in the C-H sigma bond. This is why they are poor ligands and their complexes are so short-lived (~100 ms maximum lifetime at 25 °C).

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

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

Current projects are aimed at answering questions such as: Can we make more stable alkane complexes? Can we do chemistry with the alkanes when they are bound? 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 some exciting results making the most stable alkane complexes observed to date using Os compounds and there is much scope to extend this chemistry to similar Fe and Ru complexes and explore the chemistry of the bound alkane.



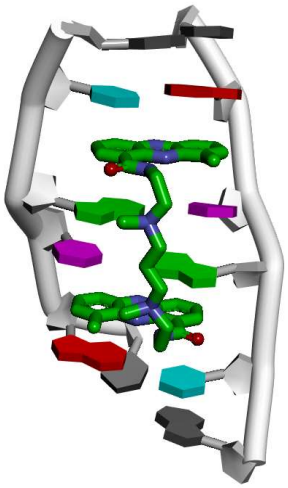
(ii) Computational design of new exotic molecules: alkane and noble gas complexes

We employ computational methods (DFT, *ab initio*) to aid the design and understanding of these fascinating compounds. Can we design then observe complexes with ligands that bind even more weakly than alkanes e.g. Xe and Kr even? For example, the recently observed cationic alkane complexes shown above were designed computationally prior to observation.[2]

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 3 components can be blended to suit the interests of students tackling the project.

1 Young, R.D.; Lawes, D.J.; Hill, A.F.; Ball, G.E. *J. Am. Chem. Soc.*, **2012**, *134*, 8294.
2 Yau, H.M; McKay, A.I; Hesse, H.; Xu, R.; He, M.; Holt, C.E.; Ball, G.E. *J. Am. Chem. Soc.* **2016**, *138*, 281.
3 Young, R.D.; Hill, A.F.; Hillier, W.; Ball, G.E. *J. Am. Chem. Soc.*, **2011**, *133*, 13806.
4 Ball, G.E.; Darwish, T.A; Geftakis, S.; George, M.W.; Lawes, D.J.; Portius, P.; Rourke, J.P. *Proc. Natl. Acad. Sci. USA*., **2005**, *102*, 1853.

(b) Anti-cancer drug-DNA interactions (in collaboration with A/Prof Larry Wakelin, A/prof Luke Hunter and Dr Don Thomas, NMR Facility)

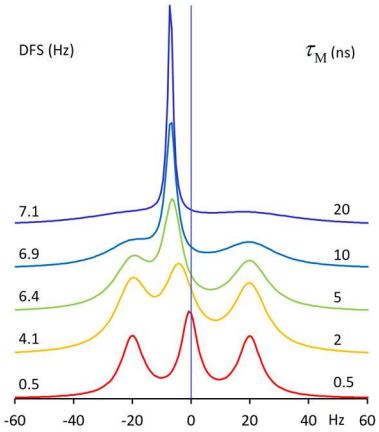


DNA presents one of the most logical and practical targets for anti-cancer therapeutics. We are investigating the binding of several mono and bis-intercalating molecules that show promise as next generation anti-cancer drugs and also the binding of clinically established drugs such as mitoxantone. The 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.[5, 6]

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

5. Serobian, A.; Pracey, C. P.; Thomas, D. S.; Denny, W. A.; Ball, G. E.; Wakelin, L. P. G. *J. Mol. Recognit.* **2020**, *33*, e2843.
6. Rowell, K.N.; Thomas, D.S.; Ball, G.E.; Wakelin, L.P.G. *Biopolymers*. **2021**, *112*, e23409.

(c) 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.

We are using various NMR techniques, including the little-known dynamic frequency shift (left) to use NMR to measure bond lengths in inorganic systems. We have recently published a study involving dihydrogen complexes,[7] which contain stretched H-H bonds and there is scope to extend this methodology to measure other, stretched bond lengths such as C-H, B-H and N-H.

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

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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

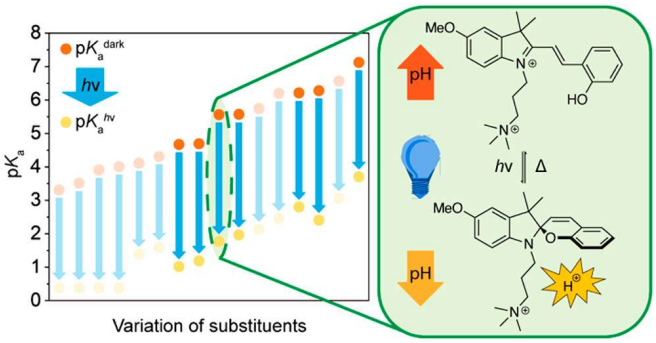
(collaborations with Prof. Tim Schmidt, UNSW, Prof. Pall Thordarson, UNSW, Prof. Dean Astumian, University of Maine, Prof. Ayusman Sen, Penn State)

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

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

Relevant publications: *J. Am. Chem. Soc.* **2020**, *142*, 20014–20020; *J. Phys. Chem. Lett.* **2021**, *12*, 1236–1243.

(b) Molecular photoswitches



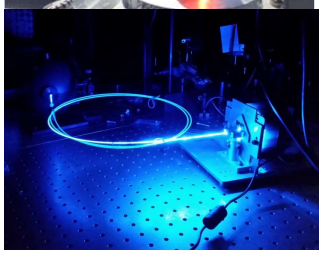
(collaboration with Prof. Joakim Andreasson, Chalmers Institute of Technology)

Some types of organic molecules can be isomerised between two forms using light. These two forms typically have very different properties, such as polarity, pK_a and reactivity. We are looking to use visible light switchable molecules to control molecular reactions, such as driving pH changes or switching ON/OFF catalytic activities.

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

Relevant publications:

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.



(c) Photoredox catalysis

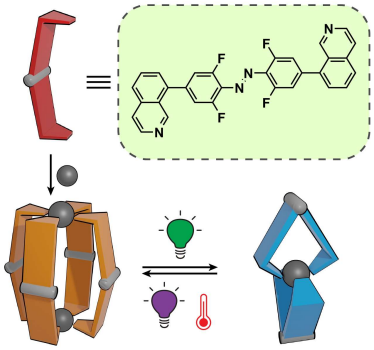
(collaboration with A/Prof. Evan Moore, UQ, A/Prof. Alex Bissember, UTas)

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

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

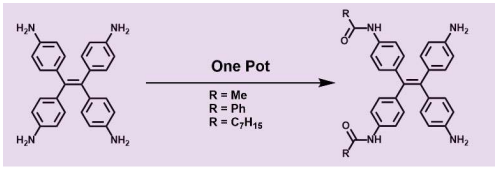
Relevant publications: *Angew. Chem. Int. Ed.*, **2020**, *59*, 9522-9526; *Inorg. Chem.* **2020**, *59*, 9135–9142 *Inorg. Chem.* ***2018****, 57, 8476–8486; Inorg. Chem.*, ***2016****, 55, 12737−12751.*

(d) Self-assembly of functional structures

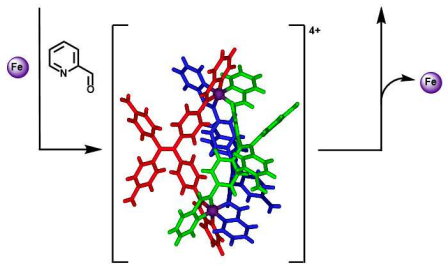


Using appropriately designed molecular components, large and symmetrical structures can be formed by "self-assembly" upon simple mixing of the different components. The resulting structures can exhibit remarkable properties, especially when constructed using transition metal complexes. This project will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

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



Relevant publications: *Angew. Chem. Int. Ed.*, **2022**, *in press; Chem. Eur. J.* **2022**, *28*, e2021044*; Chem.- Eur. J.* **2020**, *26*, 1103–1110. *Chem.- Eur. J.* **2019**, *25*, 5708-5718; *Org. Lett.*, **2017**, *19*, 4034-4037.



(e) …other projects tailored to your interests!

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

A/PROF. ALEX DONALD

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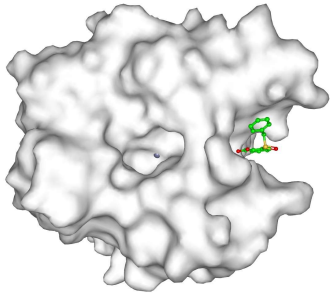
FUNDAMENTAL & APPLIED MASS SPECTROMETRY

Mass spectrometry is a core enabling technology that is used in many emerging and existing scientific fields. Dr. Alex Donald and his team are developing and applying experimental methodologies in mass spectrometry with a focus on problems in chemistry and biochemistry. We are looking for students who are interested in developing a valuable skillset in mass spectrometry and allied topics.

(a) Rapid, ultra-sensitive protein structure elucidation by mass spectrometry

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

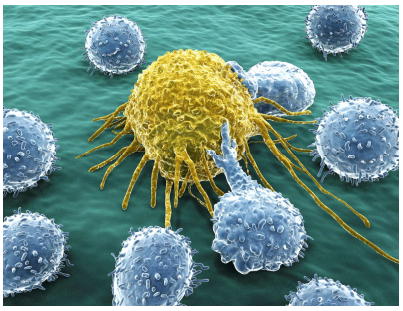


Where does the drug bind? Methods for rapidly pinpointing where small molecules bind to druggable targets are urgently needed for discovering the next generation classes of bioactive molecules.

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

(b) Single-cell chemical analysis by mass spectrometry

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



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

For single-cell chemical analysis, mass spectrometry is one of the most promising analytical techniques because it enables many different types of molecules to be rapidly detected and identified nearly simultaneously from exceedingly small sample volumes. However, matrix ion suppression is a key challenge that hinders the ability of scientists to detect the vast majority of metabolites and biomolecules in human cells. Recently, we have developed a novel, surface-selective ionization approach that enables trace chemicals to be rapidly detected from complex mixtures with minimal ion suppression using mass spectrometry.

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

(c) Cancer breathalyser

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

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

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

In this project, you will use surface enhanced ionisation mass spectrometry to rapidly detect volatile organic molecules in breath and saliva that are "signatures" for lung and breast cancer with ultrahigh sensitivity. This project is part of a longer-term thrust towards developing a high performance portable, handheld, and personal mass spectrometer for monitoring/detecting disease and detecting harmful substances in your vicinity.

DR. WESLEY DOSE

Arriving in 2022

E: wes.dose@gmail.com

MATERIALS FOR ENERGY STORAGE

We are in the midst of a battery revolution! Battery markets are growing rapidly and are set to expand even more quickly over the coming decade as we transition to cleaner energy sources and pursue net zero emissions. My research group focuses on the most pressing scientific challenges facing current and future rechargeable batteries, encompassing lithium-ion and beyond lithium-ion chemistries.

Why do batteries "die"? How can we increase their storage capacity? Can we charge in under 10 min? How do we make batteries more sustainable? Can batteries be recycled? What will the materials of the future be? Your research will seek to answer one, or more, of these questions.

The research activities in my group span several areas of chemistry, with projects available in inorganic/solid state (electrode materials), organic (liquid electrolyte), and physical (reactions at an electrode interface) chemistry. Students in the group will gain expertise in electrochemistry and a range of characterisation techniques (NMR spectroscopy, mass spectrometry, X-ray/neutron diffraction, X-ray absorption spectroscopy, electron microscopy, etc.). If you would like to learn more, feel free to contact me via email or on Twitter @DoseChemistry.

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

(a) Advanced materials for lithium-ion batteries

Lithium (Li)-ion batteries are currently the leading energy storage chemistry for use in electric vehicles (EVs) and stationary storage applications (e.g., residential- and grid-scale storage). Projects in this area will focus on understanding the chemistry of next-generation cathodes and novel electrolytes in full cells.

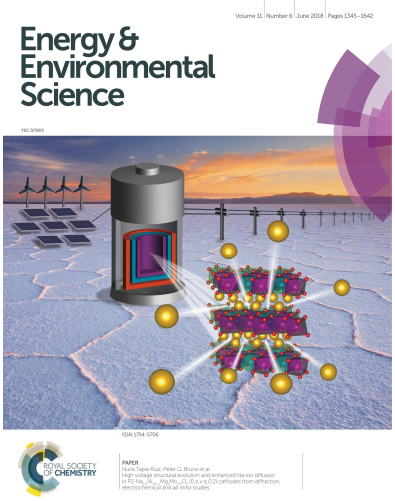
Low or no cobalt (Co) positive electrode materials

Cathode materials with low or no Co are promising next-generation materials to achieve low cost, high energy density, and more sustainable Li-ion batteries. However, these materials suffer from rapid performance fading issues that presently limit their lifetime. This project will investigate the degradation mechanisms for cathode materials from one of the following classes of materials: Ni-rich $LiNi_xMn_yCo_zO_2$ (NMC), Li- and Mn-rich, disordered rock-salt, and disordered spinel.

New Li-ion battery electrolytes

Our recent findings show that conventional Li-ion battery electrolytes are incompatible with next-generation high-energy cathodes, in particular at high voltage (https://doi.org/10.1021/acsenergylett.2c01722). This project will seek to understand the degradation of conventional electrolytes and develop new electrolytes that are mutually compatible with next-generation cathodes and next-generation anodes, while also having appropriate physical properties (i.e., viscosity, conductivity).

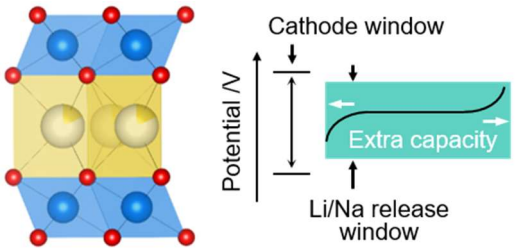
(b) Beyond lithium-ion batteries



Concerns about the future cost of lithium, due to increasing demand, are driving battery research into new chemistries beyond Li-ion. Sodium (Na)-ion batteries are a front-runner because of the relative abundance of raw materials, their environmental-friendliness, safety, and low price (https://doi.org/10.1039/C7EE02995K). These projects will tackle the most pressing issues limiting the storage capacity and long-term performance of Na-ion batteries.

Sodium ion inventory

The low sodium content of best in class Na-ion cathode materials and irreversible sodium trapping reactions at the anode severely limit the energy density of current Na-ion batteries (https://doi.org/10.1016/j.coelec.2021.100827). In this project we will discover new sodium source materials that increase the sodium inventory, and hence energy density, of the full cell. Further, we will elucidate the underlying mechanisms leading to device improvement.



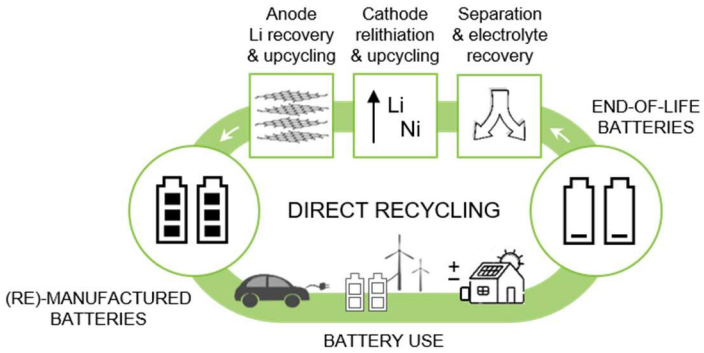
New Na-ion battery electrolytes

Innovation in electrolytes for Na-ion batteries is at present quite limited. This project will untangle the reaction mechanisms causing electrolyte degradation and design new electrolyte solutions with a particular emphasis on high-voltage stability.

Fast charging

Fast charge of batteries (e.g., charge in <10 min) is a critical challenge that must be addressed to ensure widespread adoption of batteries into certain markets, such as EVs. Present-day high-energy batteries are unable to achieve this without significant degradation of the battery performance. In this project, we will explore the main limitations for fast charge in the context of Na-ion full cells. We will use an approach combining cell construction, various testing conditions, and extensive materials characterisation.

(c) Recycling of lithium-ion batteries



The number of large Li-ion battery modules, as in EVs and residential- and grid-scale storage, reaching the end-of-life (EOL) is currently small. But as these markets grow this will soon exceed several thousand per year. This necessitates the development of safe, economic, and environmentally sound processes to reuse or recycle the materials contained within Li-ion batteries, many of which are considered critical and/or high value resources. This project seeks to explore new physical, chemical, and electrochemical processes for reuse, recycle, and up-cycle of materials extracted from EOL Li-ion batteries.

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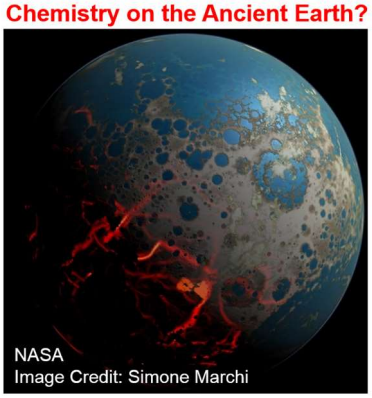
ORIGINS OF LIFE CHEMISTRY RESERACH

Chemistry plays a central role towards understanding the origins of life on Earth. ***My group seeks to develop experimental and theoretical models for understanding the potential chemistry that may have occurred on the Earth soon after its formation.*** Accomplishing this task requires a team with members who possess diverse expertise in synthetic organic, physical, analytical and biochemistries, aided by close collaborations with geo- and theoretical chemists. ***We are particularly interested in developing and understanding the chemical evolution of reaction networks that start from simple conditions (i.e., small molecules thought to be available on the early Earth) and which yield complex mixtures that contain molecules of interest, such as amino acids, ribonucleotides and their precursors.*** From these humble beginnings, the further exploration of reaction network mechanisms for RNA and peptide polymerization can allow us to understand how Darwinian evolution may have come to take over chemical evolution.

Chemistry on the Ancient Earth?

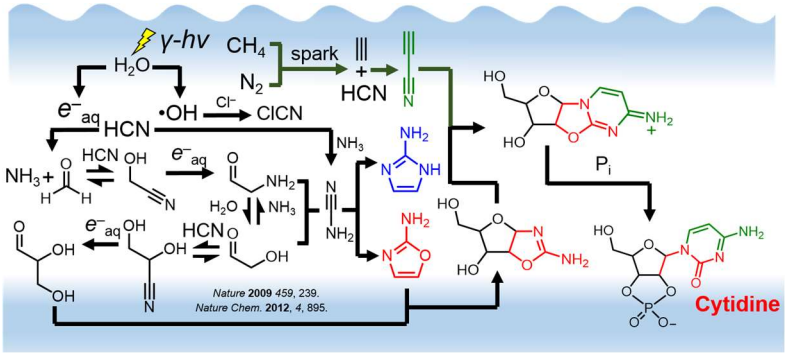


I am a new Lecturer starting in the School of Chemistry ready to take on students. Students may have potential opportunities to collaborate with and visit scientists from NASA Astrobiology labs in the US, as well as researchers from the Earth-Life Science Institute at the Tokyo Institute of Technology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

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

(a) Engineering Radiolytically Driven Reaction Networks

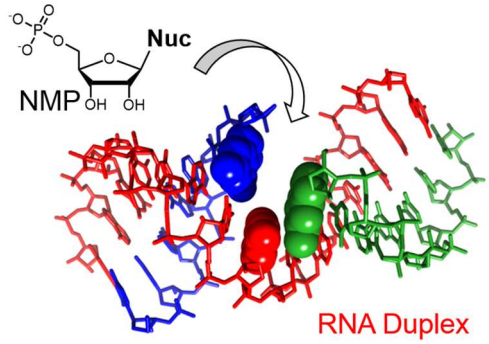
The need to make, measure and model complex reaction networks, especially those that give rise to hypothetically relevant prebiological compounds like ribonucleotides and amino acids, is fundamentally important for addressing the chemical mysteries shrouding life's origins. The goal of this project is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



understanding and engineering chemical evolution of complex mixtures in the laboratory that could have happened on the early Earth.

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

(b) Understanding the Thermodynamics of Nonenzymatic RNA Replication

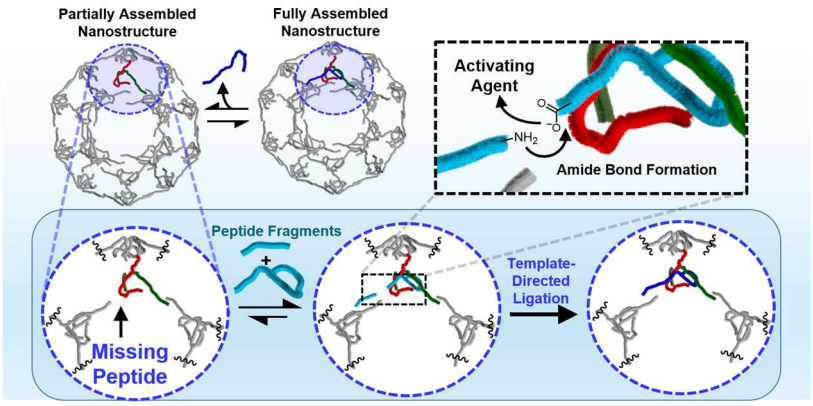


RNA is often hypothesized to be among the first genetic polymers to have arisen abiotically from chemical evolution on the early Earth. The template-directed replication of RNA – without the aid of modern enzymes – offers a mechanism by which Darwinian evolution may have originally initiated. The objective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

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

(c) Testing Possibilities for Template-Directed Peptide Synthesis

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



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

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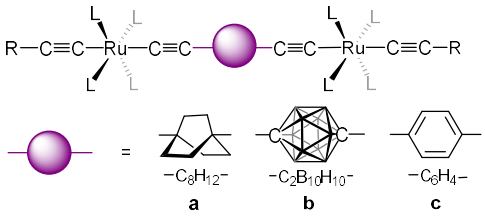
SYNTHETIC ORGANOMETALLIC CHEMISTRY

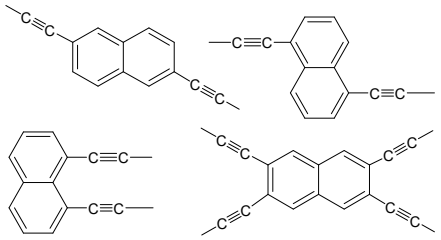
- Research in the Field group is centred around synthetic organometallic chemistry:
  - Development of organometallic catalysts that are able to activate small molecules (such as N_2, CO_2, CH_4 *etc*), and to functionalise organic hydrocarbons (CH_4, ethylene, acetylene *etc*) to make value-added products 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.

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

(a) Organometallic Polymers

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



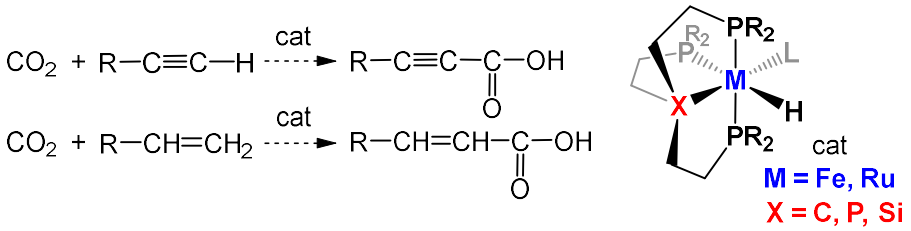


The majority of alkyne-bridged organometallic polymers use linear aromatic spacer units as the bridge between metal centres. We are interested in introducing bridges based on naphthalenes and other aromatic systems as well extending the oligomers to 2- and 3-dimensional networks.

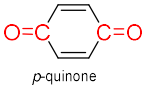
(b) The Organometallic Chemistry of Carbon Dioxide

Carbon dioxide reacts with many organometallic compounds to give products in which the CO_2 is incorporated into the metal complex. We are exploring new ways to trap and capture CO_2 and new alternate uses for this wasted and environmentally dangerous compound.

There have been reports in the literature of *catalytic* activation of CO_2 to yield formic acid H-COOH (by hydrogenation), acrylic acids RCH=CH-COOH (by reaction of CO_2 with ethylene and terminal alkenes), propiolic acids RC≡CCOOH (by reaction of CO_2 with acetylene and terminal alkynes), and carbonates (by reaction of CO_2 with epoxides). We are exploring the ability of new iron(II) and ruthenium(II) phosphine complexes that we can prepare in the lab to catalytically activate CO_2 and to produce "value-added" compounds using CO_2 as a 1-carbon starting material.

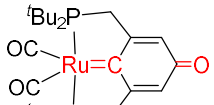


(c) Metal-to-metal communication through cross-conjugated frameworks (with Dr Martin Peeks)

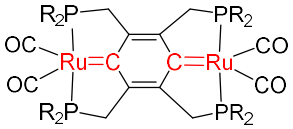


p-quinone

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 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.



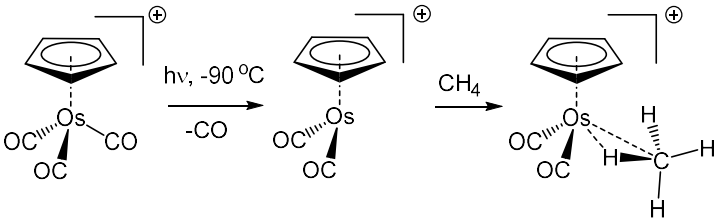
metallaquinone



dimetallaquinone

(d) Alkane binding to metals (with Associate Professor Graham Ball)

Alkanes are amongst the most stable and unreactive classes of organic compounds, and we have been studying the binding of alkanes to metals. Binding an alkane is the first step to activation of a C-H bond so that it can react with other reagents to make a substituted alkane. We are studying the key short-lived intermediates where one of the C-H bonds in an intact alkane molecule is bound to a metal.



Current projects are aimed at trying to make more stable alkane complexes and then doing chemistry on the alkanes when they are bound. We have been working with cationic metal complexes of Re and Os and we need to extend the study to complexes of Ru and Fe. The approach so far has been to generate a reactive metal species at low temperature by splitting off carbon monoxide from a metal carbonyl compound with UV light, then letting the metal react with an alkane. We characterise the compounds using NMR spectroscopy.

Selected publications from the group:

1. Dinuclear Acetylide-bridged Ruthenium(II) Complexes with Non-aromatic Spacers. Surabhi Naik, Synøve Ø. Scottwell, Hsiu L. Li, Chanel F. Leong, Deanna M. D'Alessandro, Leslie D. Field, *Dalton Transactions*, **2020**, *49*, 2687–2695. DOI: 10.1039/C9DT04856A.
2. Fe(0)-Mediated Reductive Disproportionation of CO_2. Peter M. Jurd, Hsiu L. Li, Mohan Bhadbhade, Leslie D. Field, *Organometallics*, **2020,** *39*, 2011−2018. Published online at dx.doi.org/10.1021/acs.organomet.0c00175.

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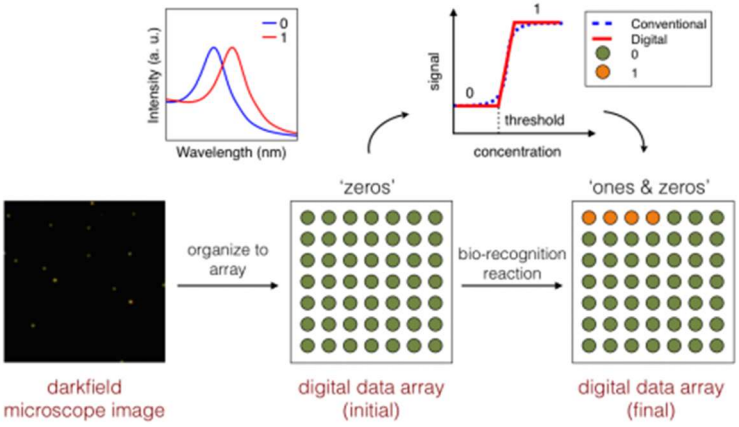
Australian Centre for NanoMedicine

SMART MATERIALS AND SURFACES

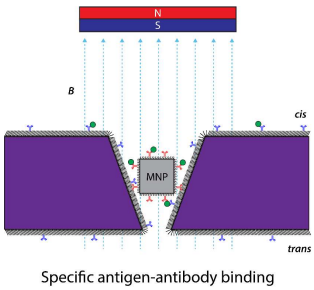
Our research group specializes in using self assembled monolayer or other surface modification technique to provide surfaces with unique functionality. The surfaces are the base upon which we build functional devices from nanscale component including polymer, protein, nanoparticles, and porous material.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

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



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

Detection of Single Biomolecules using Magnetic Nanoparticles and Nanopore Sensors

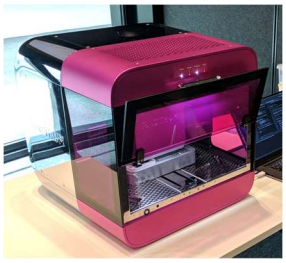


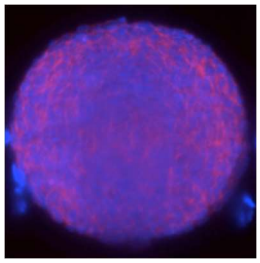
Specific antigen-antibody binding

A typical biosensors detects many molecules to give the concentration of species. Nanopores, which are commonly proposed for DNA sequencing, can detect single molecules and give concentration of species by counting many single molecules. This avoids the need for calibration however, detection limits are not as low as one expects because of the

time taken for the molecules to find the nanopores. We have solved this problem by developing a new type of nanopore, referred to as a nanopore blockade sensor. In this system, antibody magnetic nanoparticles capture the analyte of interest and brign it to the nanopore. The nanopmodified nanoporesarticle then blocks the nanopore to give a single molecule measurement. An additional benefit is the nanopore blockade sensors can operate in complex biological fluids. This projest will involves developing the next generation of this exciting single molecule sensor.

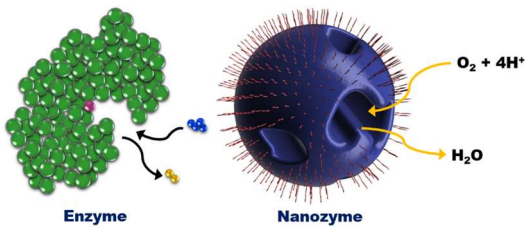
3D printing of cells for improved tumour models and drug assays **(in collaboration with Australian Centre for NanoMedicine)**





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

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



Electrocatalysts are important is applications as broad as fuels cells to sensors to production of fine chemicals. There are however a clear differences between a man made metallic electrocatalyst and a biological catalyst (an enzyme). In man made catalyst the catalytic sites are on the surface of the particle and the entire particle is conducting. However recent work in *Science* suggests catalytic sites in depressions may in fact be more active. In depressions or clefts are where most catalytic sites are located in enzymes. In this way the catalytic site is separated from the reactant solution which allows the chemical environment to be different from the bulk solution and the site to be protected from other species in solution. In this project we will synthesize catalytic nanoparticles for the oxygen reduction reaction that mimic enzyme structure by having the catalytic sites buried inside the particle but accessible via a small channel. Hence this work will focus on making core-shell nanoparticles, electron microscopy characterisation and performing electrocatalytic experiments with them.

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The true impact of fluorinated compounds in the atmosphere

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

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

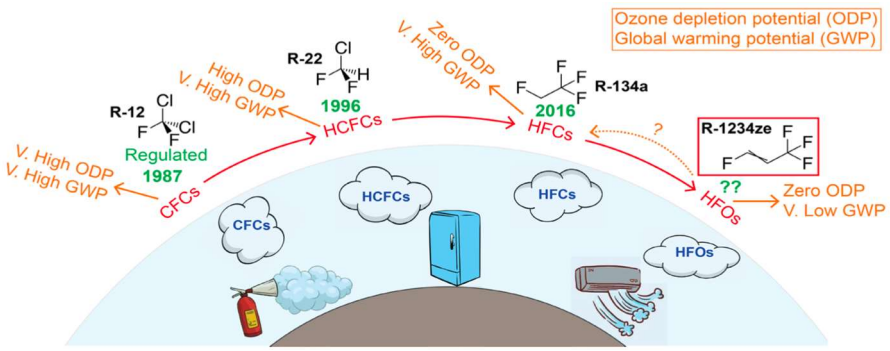
Hydrofluorocarbons (HFCs) are the replacements to the chlorofluorocarbons (CFCs) and hydrochlorofluorocarbons (HCFCs). They have no ozone depletion potential yet still present an enormous risk to the environment as powerful global warming agents. These HFCs have a high infrared activity and long atmospheric lifetimes (decades to centuries) leading to global warming potentials (GWPs) up to 10s of 1000s of times worse than CO_2. 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

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. These results re-evaluate the 'effective' GWP to one in the 100s and also account for a detected and increasing, but otherwise unexplained, source of CHF_3 in the atmosphere.



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

(b) Waste Anaesthetic Gas Destruction (with Dr Albert Fahrenbach)

General anaesthetics are typically highly fluorinated ethers with GWPs that are 1000s of times greater than CO2. Conventionally, these potent greenhouse gases are exhaled by the patient into a hospital's exhaust system and into the atmosphere where they represent over 50% of the carbon(-equivalent) footprint of operating theatres.

We have partnered with NSW Health to study photochemical options for destroying these greenhouse gases before they are exhausted from the operating theatre. We will develop photochemical reactors that will convert oxygen (O_2) and water (H_2O) in air into O atoms, ozone (O_3) and hydroxyl radicals (OH) that will rapidly decompose the target anaesthetic gases.

This project will study the photochemistry and reaction products to assess if any small, high GWP hydrofluorocarbons are formed, before deploying a custom reactor to the exhaust of an anaesthetic machine in a real operating theatre environment.

Drs Hansen and Fahrenbach scrubbed up to enter the operating theatre.

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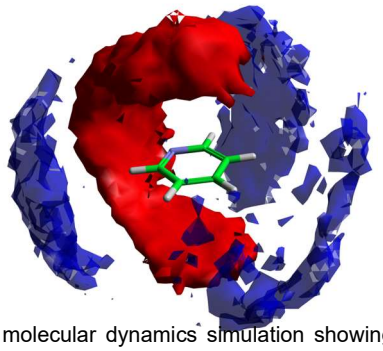
MECHANISTIC AND PHYSICAL ORGANIC CHEMISTRY

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 use d c 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.

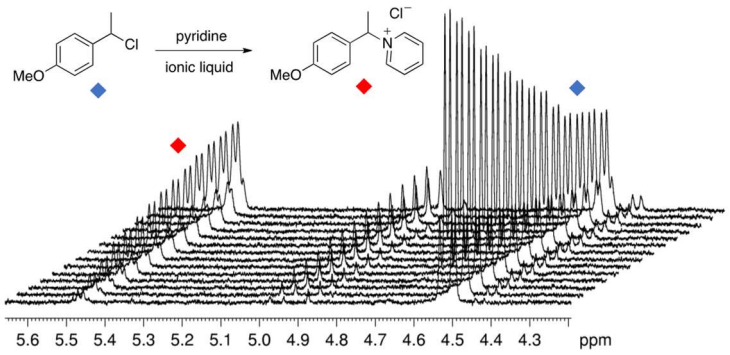
a) Ionic liquid effects on organic reactions: understanding solvation, designing better solvents and getting the reaction outcomes you want.[1] (collaborators include Dr Ron Haines & Prof. Stuart Prescott, UNSW; Prof.'s Anna Croft & Christof Jäger, University of Nottingham; Prof. Bill Price, Western Sydney University; 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**.

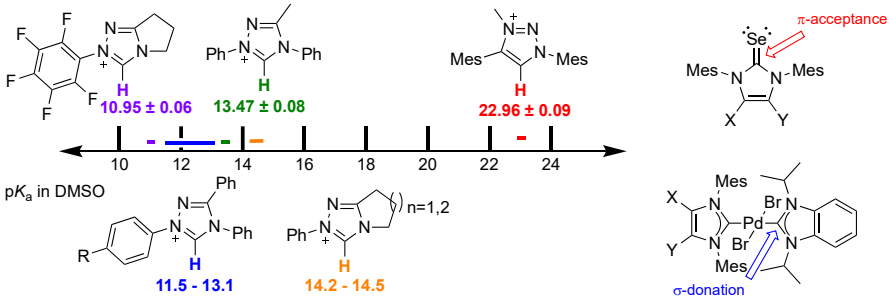
The project would involve kinetic analyses using NMR spectroscopy to monitor the progress of reactions, along with synthetic organic and analytical chemistry. Importantly, it can be readily tailored to either the physical and analytical aspects, with the opportunity to focus on methods to measure interactions 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]

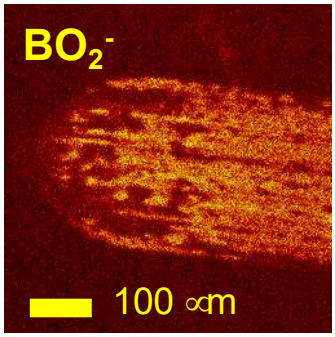
N-Heterocyclic carbenes, have significant roles in both organo- and organometallic catalysis, however some carbenes are effective for some processes but not for others; the origin of this is not well understood. This project aims to relate the structure and chemical properties of carbenes to catalytic 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. M. D. Coney *et al.*, *J. Org. Chem.* **2022**, *3*, 1767; A. Gilbert *et al.*, *J. Phys. Org. Chem.* **2021**, *34*, e3217; *Org. Biomol. Chem.* **2020**, *1*, 5442; **2019**, *17*, 675 & 9336; D. C. Morris *et al. Phys. Chem. Chem. Phys.* **2021**, *23*, 9878; 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; K. S. Schaffarczyk McHale *et al.*, *ChemPlusChem*, **2019**, *84*, 465, 534 & 9243, **2018**, *83*, 1162. 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.* **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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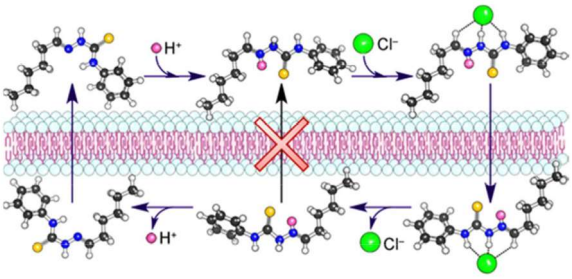
COMPUTATIONAL CHEMISTRY AND BIOMOLECULAR SIMULATIONS

We develop and apply computational chemistry methods to elucidate the mechanisms underlying many processes in synthesis and in biochemical systems (https://sites.google.com/view/mmg-unsw/home). This enables us to design improved chemical reagents, drug molecules or enzymes that our experimental colleagues can test or implement in practical applications. Topics of particular interest include, but are not limited to drug design, solvent effects and supramolecular chemistry. We work closely with experimental groups (here at UNSW and from overseas) so projects can be tailored to include an experimental component if desired. The following outlines several representative projects but feel free to get in touch to discuss your interests. No background beyond 2nd year physical chemistry is assumed.

(a) Anionophores as novel anti-cancer agents

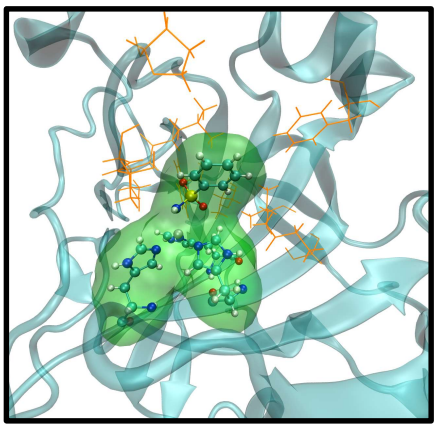
Anionophores are molecules that bind anions, most commonly through hydrogen bonding. Recent studies have revealed that these molecules can also perturb the ionic gradient in cells by transporting anions across cell membranes thereby leading to cell death (see for example, *Nature Chemistry* **2017**, *9*, 667). To further develop their potential as anti-cancer agents, we would like to simulate the binding and transport process for several families of anionophores. In this project, you will learn how to carry out electronic structure calculations and classical molecular dynamics simulations to determine the free energy barriers for the transport of a ligand across the cell membrane. This project will help establish the molecular pre-requisites for anion transport that will facilitate the design of more effective anion transporters.



(b) Understanding isoform selectivity of carbonic anhydrase inhibitors [In collaboration with A/Prof Alex Donald (UNSW) and Prof Claudiu Supuran (Florence, Italy)]

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 that perform important regulatory functions and has 12 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. (above: crystal structure of a CA inhibitor in the enzyme active site). The student will learn advanced techniques such as quantum mechanics/molecular mechanics (QM/MM) methods developed in the group to study enzymes and large macromolecules.[1,2]

(c) Accelerating quantum chemistry calculations

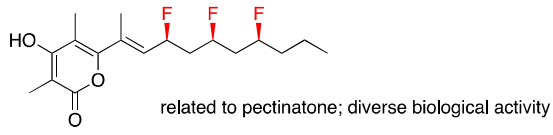
One of the key achievements in modern quantum chemistry is the development of highly accurate methods that can rival experiments. However, the computational cost (CPU hours, memory requirements) is so high that many of these methods are limited to model systems composed of several tens of atoms.
This project aims to develop an approximation based on the many-body expansion method (see equation below) to accelerate the calculations of interaction energies between molecules with their environments such as solvents, enzyme active site and surfaces.

Preliminary work in the group has indicated that this approach can lead to a **20-fold reduction** in computing time (e.g. months to days).[3] This project is ideal for a student interested in quantitative and data analysis and willing to pick up some computer programming.

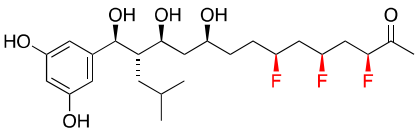
$$E = \sum_{i=1}^{N} E_i + \sum_{ij} \Delta E_{ij} + \sum_{ijk} \Delta E_{ijk} + \ldots..$$

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

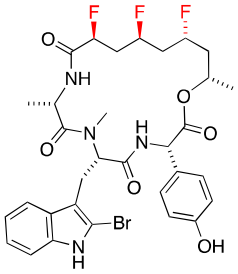
Fluorination is often used by medicinal chemists to impart structural rigidity and/or tune the lipophilicity of drug molecules. This project will use computational techniques (e.g. docking, quantum chemical and molecular dynamics simulations) to determine the 3D shapes, logP values and protein-binding ability of a variety of fluorinated bioactive molecules.[4] Examples of medicinally-relevant targets that are currently of interest within the Hunter group are shown on the left. There will also be an opportunity in this project to validate some of the computational predictions through synthesis.



related to pectinatone; diverse biological activity



related to baulamycin; antibacterial activity



related to jasplakinolide; anti-cancer activity

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3. Chen. J.; Chan, B.; Shao Y.; **Ho, J.** How accurate of approximate methods at modelling solute-solvent interactions in solvated clusters? *Phys. Chem. Chem. Phys.* **2020**, *22*, 3855.
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 # = former honours student in the group

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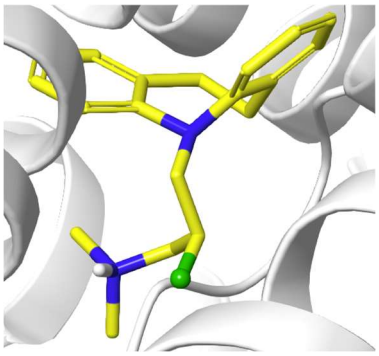
MEDICINAL ORGANIC CHEMISTRY

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.

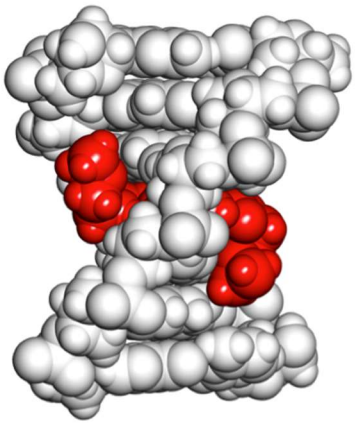
(a) "Molecular origami": using fluorine to control the shapes of bioactive molecules
(in collaboration with Dr. Junming Ho; Dr. Angela Finch [SOMS]; Dr. Nicola Smith [SOMS])

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])

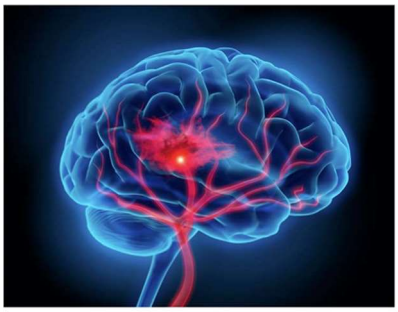
Cancer is a common disease that kills 1 in 3 of us in the Western world. Chemotherapy is the principal treatment for metastatic cancer, but its effectiveness is limited by the resistance that tumour cells can develop to many conventional drugs. We are developing new drugs that will bind to DNA and weld 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]

[1] Y. Lizarme-Salas, A. D. Ariawan, R. Ratnayake, H. Luesch, A. Finch, L. Hunter, "Vicinal difluorination as a C= C surrogate: an analog of piperine with enhanced solubility, photostability, and acetylcholinesterase inhibitory activity," *Beilstein J. Chem.* **2020**, *16*, 2663.

[2] A. Lawer, L. Hunter, "Controlling γ-peptide helicity with stereoselective fluorination," *Eur. J. Org. Chem.* **2021,** 1184.

[3] A. D. Ariawan, F. Mansour, N. Richardson, M. Bhadbhade, J. Ho, L. Hunter, "The effect of vicinal difluorination on the conformation and potency of histone deacetylase inhibitors," *Molecules* **2021**, *26*, 3974.

[4] S. Chen, Y. Ruan, J.L. Lu, L. Hunter, X. G. Hu, "Diastereoselective synthesis and conformational analysis of 4, 5-difluoropipecolic acids," *Org. Biomol. Chem.* **2020**, *18*, 8192.

[5] C. Au, C. Gonzalez, Y. C. Leung, F. Mansour, J. Trinh, Z. Wang, X. G. Hu, R. Griffith, E. Pasquier, L. Hunter, "Tuning the properties of a cyclic RGD-containing tetrapeptide through backbone fluorination," *Org. Biomol. Chem.* **2019**, *17*, 664.

[6] A. Lawer, J. Nesvaderani, G. M. Marcolin, L. Hunter, "Synthesis and biochemical characterisation of fluorinated analogues of pepstatin A and grassystatin A," *Tetrahedron* **2018**, 74, 1278.

[7] N. L. Richardson, L. J. O'Malley, D. Weissberger, A. Tumber, C. J. Schofield, R. Griffith, N. M. Jones, L. Hunter, "Discovery of neuroprotective agents that inhibit human prolyl hydroxylase PHD2," *Bioorg. Med. Chem.* **2021**, *38*, 116115.

[8] G. Surjadinata, L. Hunter, L. Matesic, G. Pascali, "Analytical-scale synthesis of aryl-SF_4Cl via flow microfluidic technology," *J. Flow Chem.* **2021**, *11*, 107.

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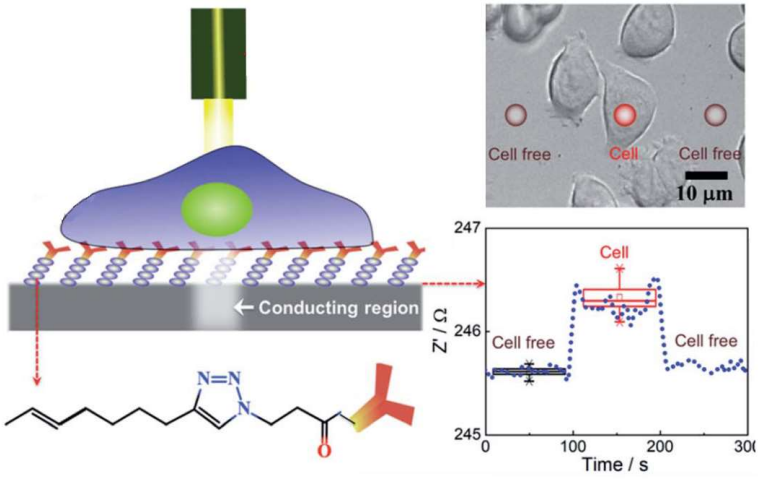
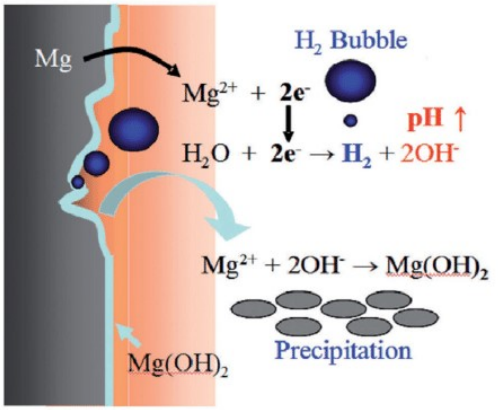
Electrochemistry of living cells and materials

My research is centred around advancing electrochemical techniques toward enabling smarter design of materials as well as finding new ways to communicate with cells. Cells communicate via electrochemical mechanisms. Our ability to use technology to talk to cells in their native "electrochemical" language offers potential for new understanding and treatment of disease. Our ability to record and analyse very small currents and voltages that are linked to chemical reactions allow us to get ever closer to the fundamental functions of materials and cells. We exploit electrochemistry to look into the interaction between materials, physiological environment and cells to help with more advanced design of biosensors and biomaterials. New members will work within the Smart Materials and Surfaces research group led by Scientia Prof. Justin Gooding. Following projects are the specific areas of interest while other projects of mutual interest will also be considered. It would be great to work with Honours students on the following projects:

(a) Light activated electrochemistry (in collaboration with Professor Justin Gooding)

Localising electrochemistry to small regions on a large surface is of particular interest among recent advances in electrochemistry since it enables screening of single cells in a non-invasive manner. This allows cells response to drugs to be studied individually and also opens a new window to advancement of bioelectronics. Among the current approaches to localised electrochemistry, the Light Activated Electrochemistry (LAE) technique, that has been developed to great depth by the Smart Materials and Surfaces group, offers unique advantages. The activation of specific areas of a surface by light is based on light exciting photoelectrons from the valence band to the conduction band of a semi-conducting silicon electrode that is in depletion. The technique has been utilised for the detection of ion release from single cells, combined with fluorescence microscopy to show how the cells respond to drug treatment. Further work in this area will involve using LAE platform to record intrinsic noise that is generated by cells for a multimodal characterization as well as utilising the platform for modulation of cell's functions through application of external signals.





(b) Biodegradation of implant materials

Bioresorbable metallic implants have introduced a new paradigm in regenerative surgery treatment, in particular as alternative to conventional cardiovascular stent and bone fixation materials. For the implant to be successful, it requires to degrade and dissolve in the surrounding media gradually as the supported tissue heals. The degradation rate needs to be fine-tuned to match the rate at which the tissue regains mechanical stability.

New projects in this area will investigate electrochemical techniques and sensors to monitor the onset and kinetic of degradation and the various physico-chemical processes taking place in real time. Surface modifications are often performed on the biomedical implants to improve chemical/electrochemical stability, wear resistance, surface texture and biocompatibility. Of particular interest is electrochemical noise method to enable non-intrusive and real time assessment of kinetic and thermodynamic of electrochemical reactions taking place at the surface of implant material. For realistic simulation of the degradation properties, a range of environmental parameters, e.g. load and cycles, ions/electrolyte, proteins, cell adhesion, mobility, temperature etc, will be taken into account to more closely mimic a biological environment.

(c) Electrochemical noise as a platform for sensing

Current electrochemical sensors rely on three main protocols for data acquisition namely, amperometry, potentiometry and impedimetry. Electrochemical noise, unlike the three conventional techniques, relies on the naturally occurring chemical processes for data acquisition without the application of any external bias voltage or current and yet it yields all three amperometric, potentiometric and impedimetric information in a single measurement. This brings about new capabilities in biosensors. The intrinsic noise is originated from any physical and/or chemical phenomenon that changes the equilibrium state at the electrode/electrolyte interface and can cause fluctuation of current and potential. For example, adsorption of charged particles onto the electrode surface changes the electrical state at the electrical double layer that is manifested as a fluctuation in potential and can be experimentally measured. In the absence of external bias current and voltage, the electrode surface will re-establish equilibrium to balance out the extra charge and this will cause a fluctuation in current. This current fluctuation can also be measured. The aim for new projects in this space is to explore the implementation of electrochemical noise principle in developing biosensors with multimodal sensing capabilities.

I also welcome discussions on your project ideas around the electrochemistry and biomaterials. Feel free to send me an email or just just drop by my office in Hilmer 746.

Interested students can find more context in the following references or by contacting Dr Jamali directly

Y. Yang, F.M. Mansfeld, M. Kavallaris, K. Gaus, R.D. Tilley, J.J. Gooding, Monitoring the heterogeneity in single cell responses to drugs using electrochemical impedance and electrochemical noise, Chem. Sci. 12 (2021) 2558–2566.

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S.S. Jamali, D.J. Mills, A critical review on electrochemical noise measurement as a tool for evaluation of organic coatings, Prog. Org. Coatings. 95 (2016) 13–17.

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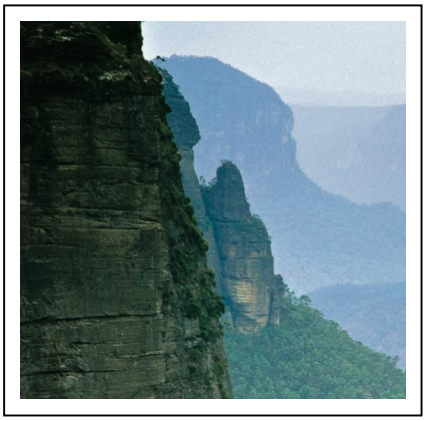
LASER PROBES OF CHEMICAL REACTIONS

- 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, Sydney U.; Jenny Fisher, U. W/gong; Chris Hansen, UNSW)

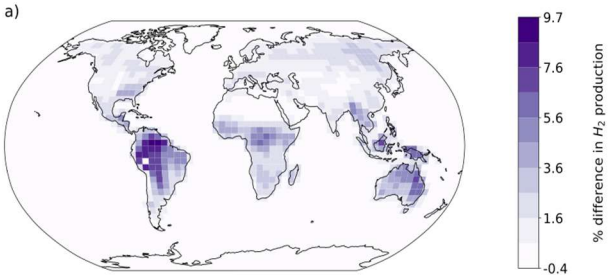


The poor state of our atmosphere is one of the most pressing issues facing society today. Everyone knows about the challenges of climate change. But did you realise that more people meet premature deaths from poor air quality than form either cancer or heart disease?

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 classes 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).

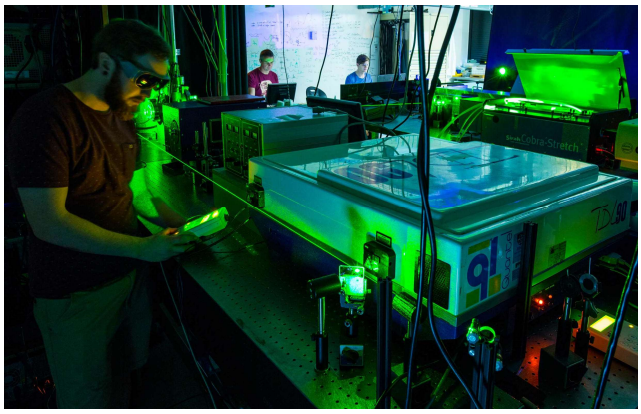


(b) Weird chemistry – reactions that just don't go where they should. (Collaborators: Meredith Jordan, Sydney U., David Osborn, Sandia National Labs, USA)

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 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.

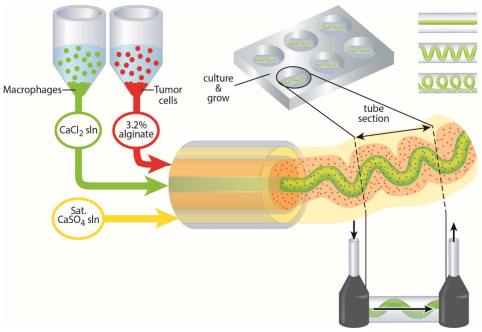

Fig. 1. Extrusion of cell-laden chemically modified alginate (*Adv. Mater., 2015*)

(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

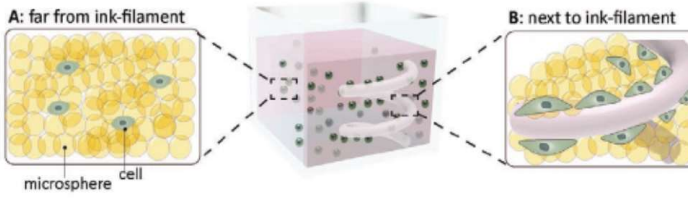

Fig. 2. Ceramic Omnidirectional Bioprinting in Cell Suspensions (Romanazzo et al., *Adv. Funct. Mater.,* 2021)

developed a novel apatite-transforming ink that can be 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.

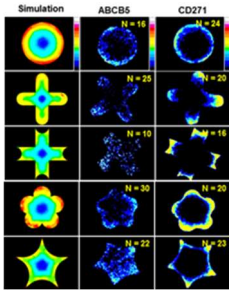

Fig. 3. Interfacial curvature will guide the activation of a stem-like state (Lee et al., *Nat. Mater.*, 2016)

(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.

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.

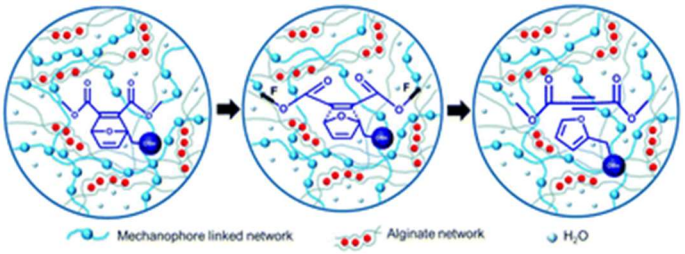

Fig. 4. Compression or tension triggers molecule release in double network hydrogels (Jayathilaka et al., Chem. Commun. 2021)

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.

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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.

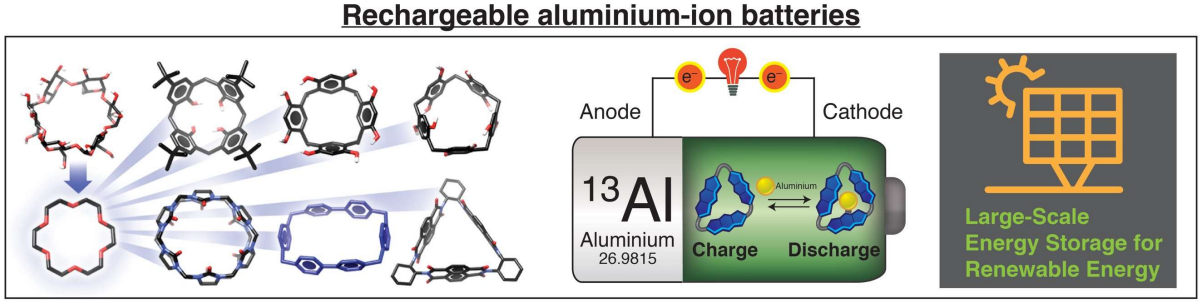

Figure 1. Graphical representation of the macrocyclic building blocks into nano-channels.

(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.

Artificial molecular dual pump

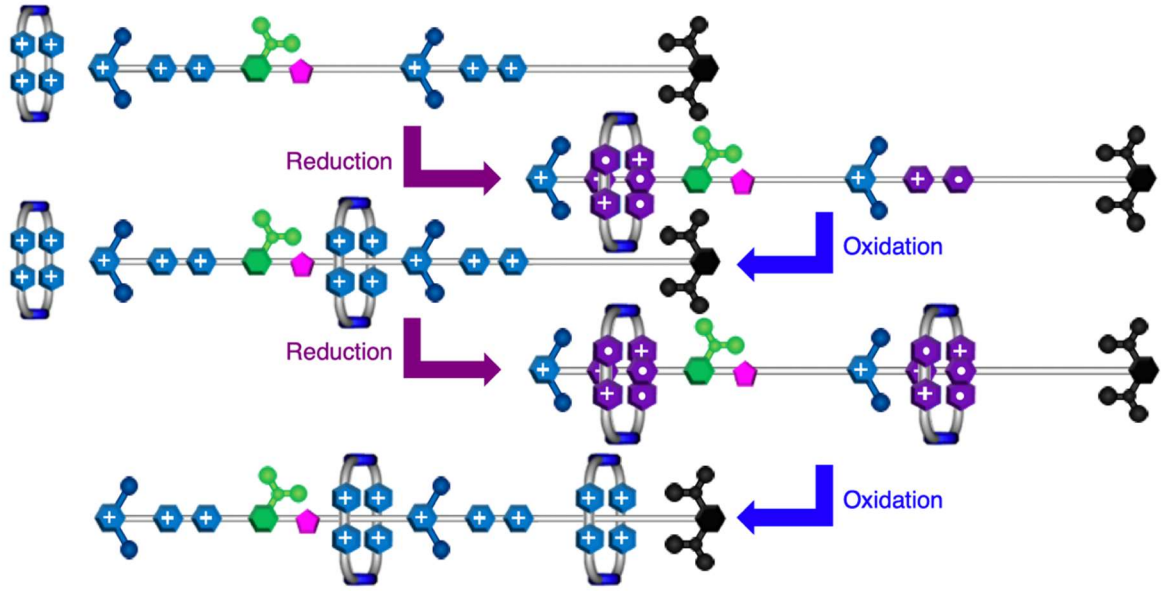

Figure 2. Structure the molecular dual pump and pumping rings onto the collecting chain chemically and electrochemically.

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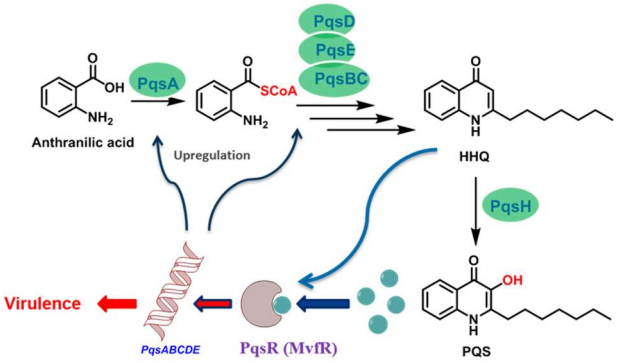
SYNTHETIC ORGANIC AND MEDICINAL CHEMISTRY

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.

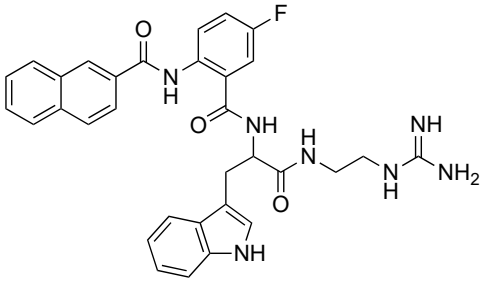
(a) DESIGN AND SYNTHESIS OF NOVEL ANTIMICROBIAL AGENTS

Quorum Sensing Inhibitors



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.

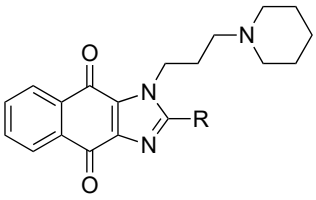
Inhibitors of Bacterial Transcription Initiation

(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.

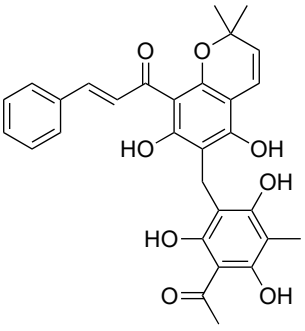
(b) DEVELOPING ANTICANCER COMPOUNDS THAT ACTIVATE GLUCOSE OXIDATION

(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 HETEROCYCLIC SYSTEMS



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

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CHEMISTRY EDUCATION RESEARCH AND GREEN CHEMISTRY SYNTHESIS

We are a new group joining UNSW in 2023, please get in contact to be part of this new adventure.

- As part of UNSW chemistry education research, our strategy encompasses inclusive learning environments, learning analytics and systems thinking for context-based learning
- Our discipline-based research centres on green chemistry and catalysis, including reaction design and mechanistic understanding
- Students with chemistry, education and other backgrounds are welcome, as diversity is key to tackling interdisciplinary challenges
- We have ongoing close collaborations with groups in the UK, Europe, the Philippines and across Australia
- Please do not hesitate to contact me to discuss your research interests and possible projects in more detail

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

(a) Promoting inclusive learning environments

(in collaboration with the University of the Philippines Open University, The Philippines)

Modern education is seeing an increase in the diversity of learners, and as educators we are exploring effective ways to address educational gaps such that all students can benefit from equitable access to quality education. To create these inclusive learning environments, we are designing proactive and flexible teaching approaches and learning resources guided by the Universal Design for Learning framework.[1] We are also interested in exploring the vast role of instructional design and learning design in improving access to quality learning resources and activities, especially in online learning environments. To inform our approaches we are evaluating accessibility by harnessing big data and the emerging field learning analytics. Through this approach, we aim to establish clear metrics to evaluate and promote inclusivity of learning environments.

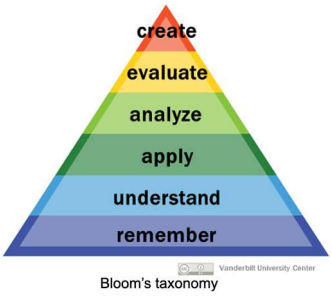
(b) Sustainability and green chemistry through context-based learning and systems thinking

(in collaboration with Dr. Shannan Maisey, 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, the impact of these activities will be evaluated based on academic performance, student satisfaction and engagement, based on shifts in students' beliefs and improvements on their perceptions) towards sustainability as influenced by the enhanced curriculum.

(c) Authentic assessment practices post COVID-19

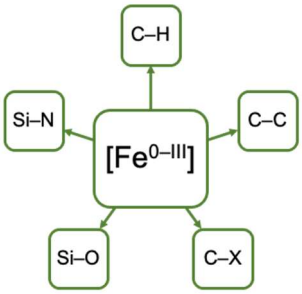


Bloom's taxonomy

(in collaboration with Dr. Siobhán Wills, UNSW and the University of Sydney)

In 2020, Universities world-wide were forced to teach and assess everything online. While all aspects of teaching and learning were impacted, end-of-semester examinations pose specific challenges due to concerns of academic integrity, question design, and technological requirements. Furthermore, the online delivery of assessment had introduced uncertainties on the authenticity of the assessment process. Together with the University of Sydney, we are investigating how online STEM examinations compare to those delivered more traditionally (paper-based) to establish where they are positioned in a continuum of authentic assessment strategies. We are analysing question design and composition to determine what impact transitioning online had on exam structure and student performance. These findings will inform recommendations for best practice in Australian STEM disciplines for authentic assessment, supported by the Australian Council of Deans of Science.

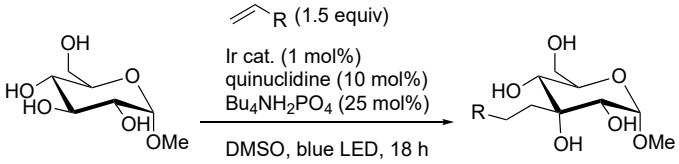
(d) Iron catalysed reactions



(in collaboration with the University of Bath, UK)

First row transition metals have found applications as homogenous and heterogeneous catalysts. In particular, iron can act as a powerful redox active catalyst for both single- and two- electron transfer processes. We are designing new iron-based synthetic methods for applications including polymerisation, intra- and intermolecular radical reactions, and main-group bond formation.[2] Our research investigates the mechanism of the catalytic cycle, aiming to identifying key reaction intermediates and understand their chemical, physical and electronic properties.

(e) Site selective photoredox catalysis



We are developing site-selective catalytic methods to transform simple sugars. These reactions use photoredox catalysts and visible light to promote carbon-carbon bond formation. The reaction mechanism is proposed to occur through the coupling of two different radical reactions. We are investigating the reaction mechanism, and how various radical species and metal intermediates interact. This is important to inform design of new, site-selective synthetic reactions of more complex sugars.

1. C. T. Reyes, G. A. Lawrie, C. D. Thompson and S. H. Kyne, "Every little thing that could possibly be provided helps": Analysis of online first-year chemistry resources using the universal design for learning framework. *Chem. Educ. Res. Pract.*, 2022, **23**, 385–407. https://doi.org/10.1039/D1RP00171J

S. H. Kyne, G. Lefèvre, C. Ollivier, M. Petit, V.-A. R. Cladera and L. Fensterbank, Iron and cobalt catalysis: new perspectives in synthetic radical chemistry, *Chem. Soc. Rev.*, 2020, **49**, 8501–8542. https://doi.org/10.1039/D0CS00969E

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COMPUTATIONAL MATERIALS SCIENCE AND CHEMISTRY FOR SUSTAINABILITY APPLICATIONS

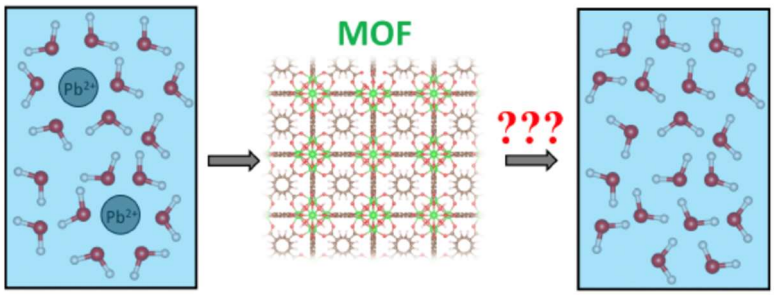
Computer simulations are an essential tool to make high-impact discoveries in fields that are crucial to our sustainable future. In general, these types of simulations allow us to calculate properties of molecules and materials at the atomic scale, which can be too difficult to be measured by experiments.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

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

Some of the projects currently available are:

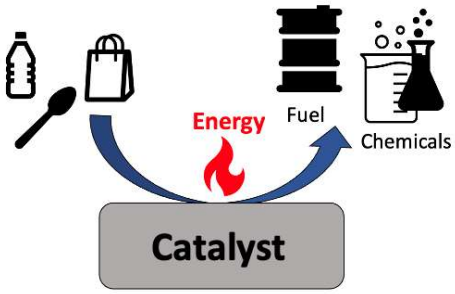
(a) Computational Design of Metal-Organic Frameworks for Clean Water Harvesting and Water Purification

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.

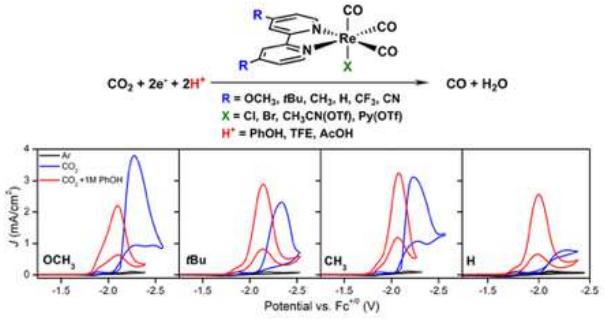


(b) Plastic Waste and Carbon Dioxide Conversion into Useful Products using Transition-Metal Catalysts

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.



CO2 conversion into liquid fuels is a promising avenue towards efficient electrical energy storage and at the same time reduction of CO2 concentration in our atmosphere. Transition metal complexes have been shown to be capable electrocatalysts for the conversion of CO2 into useful products but improvement is still needed. This project uses computational tools to design improved catalysts by testing the use of more Earth-abundant metals and studying the effect of changing the ligands and counterions.



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

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 and CO_2 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

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COORDINATION CHEMISTRY OF METAL-ORGANIC FRAMEWORKS

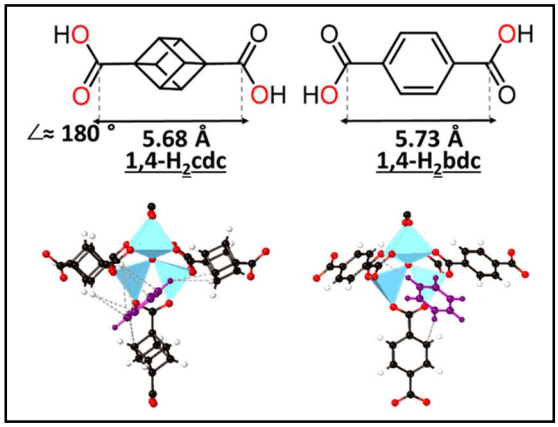
Metal-organic frameworks (MOFs) are porous coordination polymers built from the self-assembly of metal clusters and organic linkers. Through careful selection of these building blocks when designing our MOFs, materials with pre-determined properties can be synthesised. Our research area uniquely encompasses 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 students on the following projects:

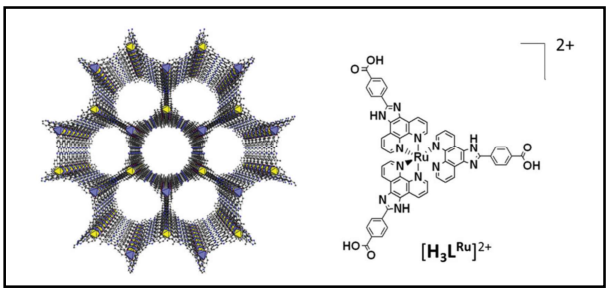
(a) 3D-Linker MOFs for separations and storage



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)

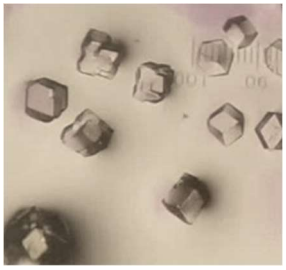
(b) Photoactive frameworks for water splitting or CO_2 reduction



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

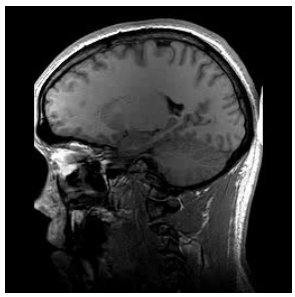
tuneable luminescence can be gained through modulation of linkers with mixed functionalities and the incorporation of mixed metals (eg. Ru and Co). This project investigates increasing the luminescent lifetimes of phenanthroline based MOFs through varying the conjugation in the MOF linker. As an added 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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CHEMISTRY EDUCATION IN THE 21ST CENTURY

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

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

Keywords: Systems thinking, Global challenges, Mastery learning

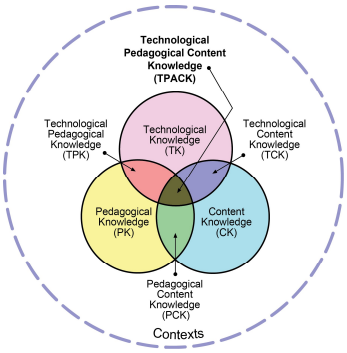
The world is currently facing unprecedented challenges which are affecting all facets of life on earth. Climate change, Sustainability and the need for Renewable energy sources and storage are challenges which have chemistry at their core. A recent article in Nature Reviews Chemistry[1] served as a call to arms for chemistry educators to integrate systems thinking into chemistry curricula at all levels to empower our students with the knowledge and skills to face these challenges. Systems thinking is about putting chemical concepts into a real worlds context and showing how atoms and molecules (and the decisions we make with what to do with them) impact people's lives and our environment. There is very litter literature which describes systems thinking in chemistry which presents many exciting opportunities for your project from exploring the challenges of integrating it into chemistry curricula to finding out how student's viewpoints develop and change with a broader view of chemistry…it's an exciting time to be alive!

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

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

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

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

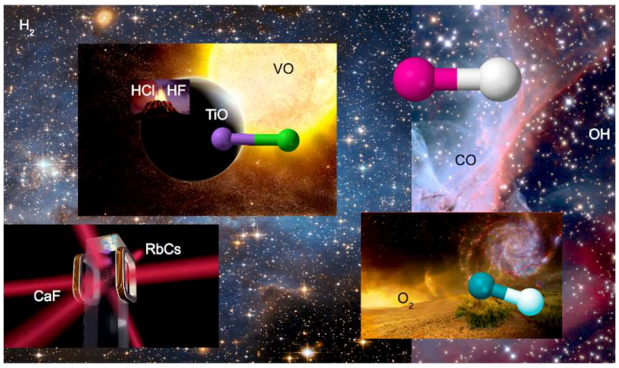


Keywords: *Digital Literacy, PCK, TPACK, Online learning, Blended Learning*

Pedagogical content knowledge (PCK) theory recognizes that beyond the teacher's own understanding and knowledge of the content theory there is a surrounding body of knowledge to do with how students learn and process information specific to the theory being taught. In the age of technology, the way we interact with students has changed. Technological pedagogical content knowledge (TPACK) is the basis of effective teaching with technology, requiring an understanding of the representation of concepts using technologies; pedagogical techniques that use technologies in constructive ways to teach content; knowledge of what makes concepts difficult or easy to learn and how technology can help students overcome difficulties[2].

How students engage with technology to learn is rapidly evolving. Like many other institutions, online learning is now one of our underpinning methods of teaching first year chemistry. What is not well understood is what strategies students are engaging to use and supplementing these materials to facilitate learning. Why are some formats preferred by students and how is this impacted by demographics? Is there potential to impact how effectively we can teach students chemistry by 'updating' our TPACK?

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



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

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

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

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

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

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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

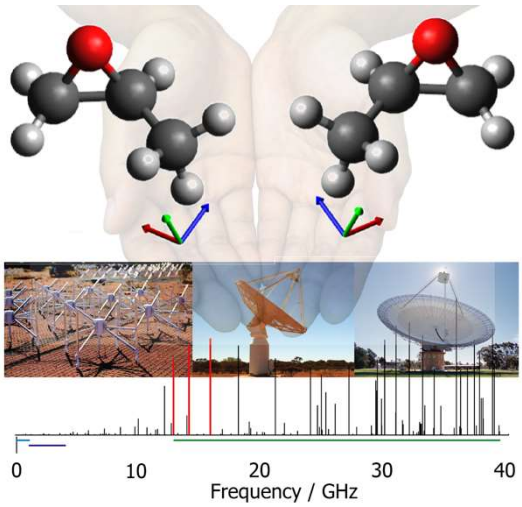
Keywords: Machine Learning, Data Science, Computational Quantum Chemistry, Supercomputers, High-throughput Calculations, Spectroscopy

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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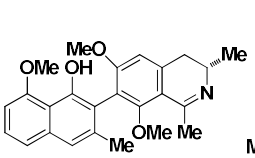
SYNTHETIC AND MEDICINAL CHEMISTRY

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

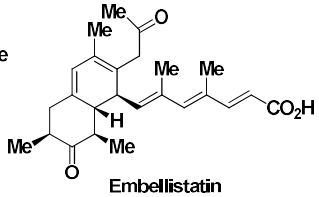
It would be great to work with Honours students on the following projects:

(a) Total Synthesis of Biologically Active Natural Products

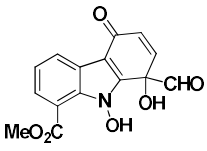
The development of efficient syntheses of biologically active natural products continues to be a major activity of the Morris group, with recent targets including ancistrotanzanine A, embellistatin and coproverdine. As syntheses of these targets are completed, work is initiated on their mode of action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



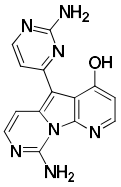
Ancistrotanzanine A



Embellistatin



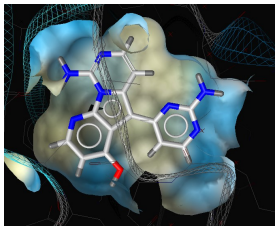
Coproverdine

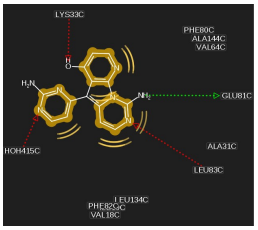


Variolin B

(b) Developing Inhibitors of RNA Splicing Kinases

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





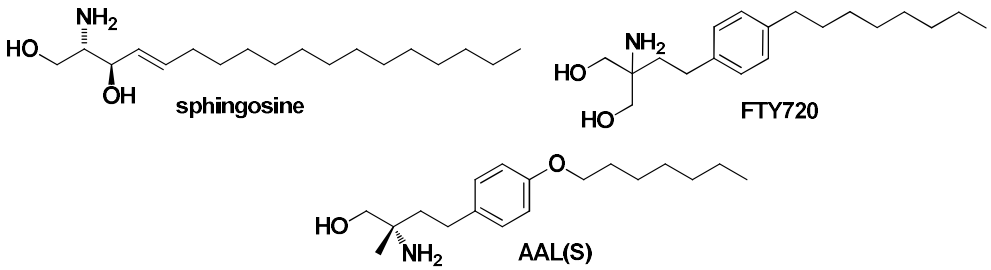
The Morris group is actively engaged in the development of small molecules that can do this, and this is achieved by targeting the protein kinases that mediate the phosphorylation. This work originated from earlier work on the synthesis of a natural product. Variolin B is a member of a unique class of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

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

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

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

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



Development of the AAL(S) scaffold will allow for analog production which along with key biological testing will provide key information towards revealing the biochemical pathways and proteins involved regulating both enzymes at a molecular level. With Prof Ammitt, work is focused on using these molecules for the development of therapeutics for the treatment of asthma, whereas with Asoc Prof Turner we are developing molecules to elucidate the role of CerS in fat metabolism (see Turner et al, Nature Communications, 2018, 9: 3165 | DOI: 10.1038/s41467-018-05613-7)

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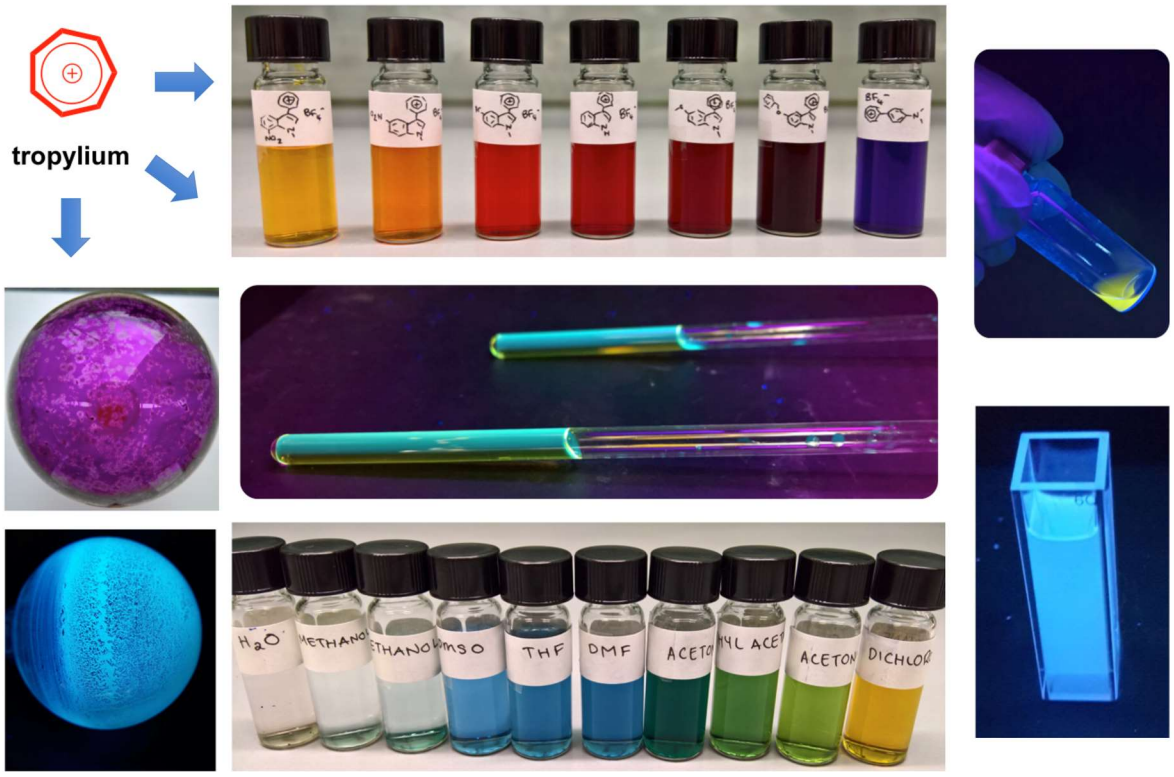
ORGANOCATALYSIS AND CHEMISTRY OF UNUSUAL MOLECULES

Nguyen's group has several Honours projects focusing on the development of novel organocatalytic systems or unusual molecules and applications of those in synthetic organic chemistry.

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

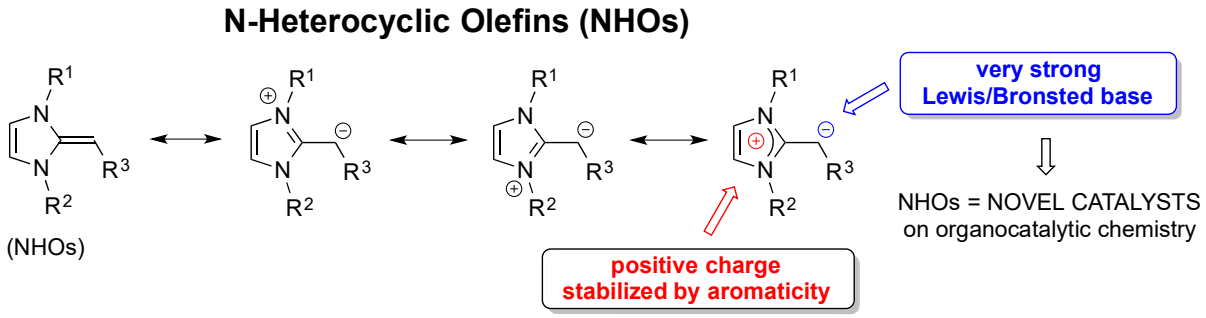
Tropylium ion is an unusual non-benzenoid aromatic system with 6π-electron 7-carbon-ring structure.[1] Recent synthetic advances by our group have made this unique species much more accessible and understood, allowing us now to start to utilize it for a wide range of applications in organocatalytic chemistry[2-5]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



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

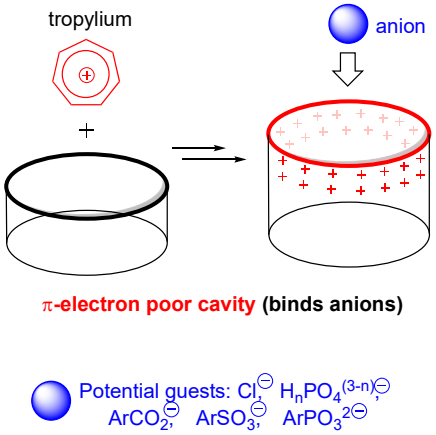
Recently, N-Heterocyclic Olefins (NHOs, see scheme) have emerged as a new class of valuable reaction promoters with interesting action mechanisms. These compounds can be conveniently produced from commercially available precursors in one step. NHOs were originally targeted as a

series of active agrochemicals in the 1970s, but they slowly revealed to be a far more interesting compound family. Due to the donating ability of the two nitrogen atoms, the exocyclic C-C double bond is very electron-rich and strongly polarized. This interesting feature of NHOs offers multinucleophilic reactivity over the ketene aminal frameworks.[6] Due to the strong nucleophilicity of the α-carbon, NHOs can act as strong Lewis/Bronsted bases.[7-9] This project will focus on synthesizing a family of NHOs, estimating their basicity and applying them as organocatalysts to promote ***environmentally friendly chemical processes***. Students are encouraged to discuss with Vinh in person about this project.



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

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



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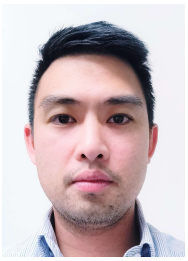
Radiochemical innovations

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

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

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



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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.

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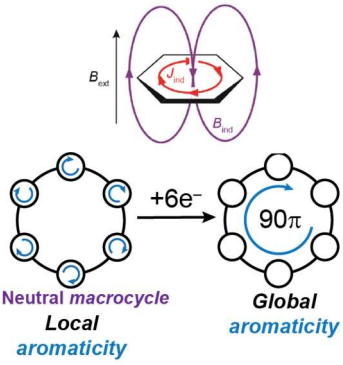
SUPRAMOLECULAR & ORGANIC MATERIALS CHEMISTRY

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:

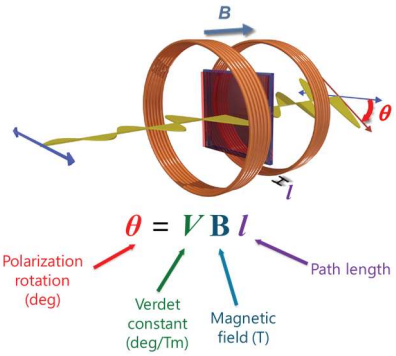
(a) Pushing the limits of π-conjugation, aromaticity, and antiaromaticity



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.

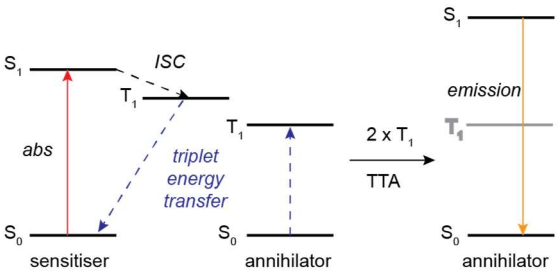
Despite the Faraday effect's ubiquity, it's actually quite weak in most materials, except some ferrimagnetic garnet materials – or that was the prevailing wisdom. Recently it's been discovered that a range of organic materials, from polymers through to liquid crystals, exhibit extreme Faraday rotation.[2]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

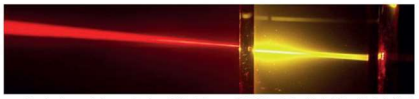
from this initial discovery is to learn *how molecular structure controls* the Faraday rotation. With that knowledge, we will be able to logically design new materials with possible applications in healthcare, self-driving vehicles, and photonics/spintronics.

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.

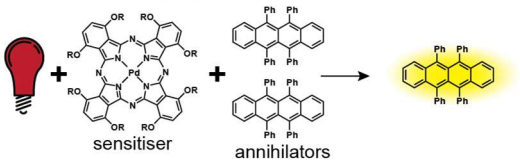
(c) Molecules and assemblies for photon upconversion (with Prof. T. Schmidt)

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

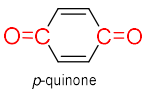


Photon upconversion requires the complex interplay of several different chromophores and their excited states. The relative arrangement of these chromophores in space, as well as their identities, is key for successful upconversion.[4]

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.

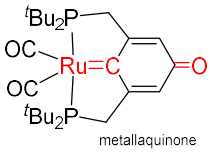
(d) Metal-to-metal communication through cross-conjugated frameworks (with Prof Les Field)

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.

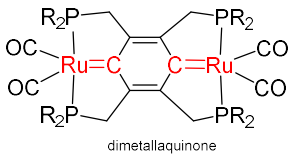


p-quinone

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.

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STRUCTURAL CHEMISTRY WITH MASS SPECTROMETRY & ION-MOBILITY

Can you envisage a world where building a brand new catalyst or an artificial enzyme is as simple as following an architectural plan for a house? At the moment this is difficult because we don't even fully understand the construction materials! Our research investigates the intrinsic properties of molecular building-blocks and their "constructed" aggregates, moving us towards the ability to draw up these molecular blueprints from scratch.

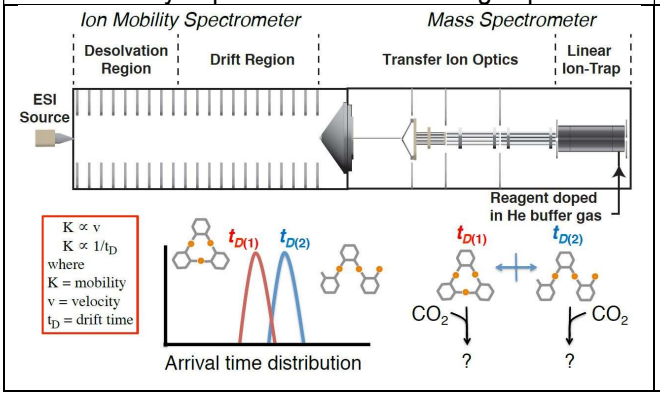
We utilize a range of cutting-edge technologies in our chemical analyses, including, but not limited to; high resolution ion-mobility spectrometry, advanced mass spectrometry, computational chemistry, combinatorial robotics and wet chemistry methods. We are interested in structure-function relationships, mechanism, theory underpinning chemical reactions and catalysis, chemical data crunching, and methodological development (for mass spectrometry and ion-mobility). Understanding the intrinsic properties of molecules, molecular building blocks and aggregates is key to realizing the bottom-up design of functional molecules and materials, and catalysts. We explore such molecular units in isolation. The end goal of this research is the rational design of efficient catalyst and enzyme-like molecules.

Unique skillset researchers will develop in the Rijs group during honours include becoming expert at:

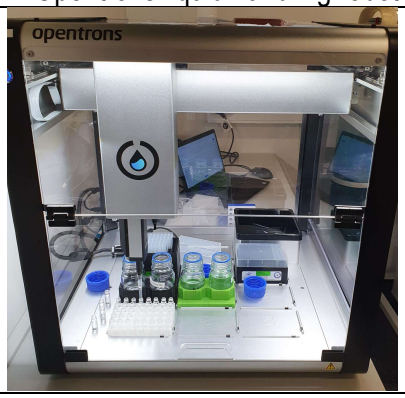
- advanced electrospray ionisation mass spectrometry and ion-mobility mass spectrometry (**A**),
- robotic preparation and analysis of solutions (**B**),
- screening of chemical data sets,
- electronic methods of computation for structure and function

No prior experience is necessary and many of these skills are currently in demand in industry.

A Ion mobility separates isomers in the gas phase



B Opentrons liquid handling robot

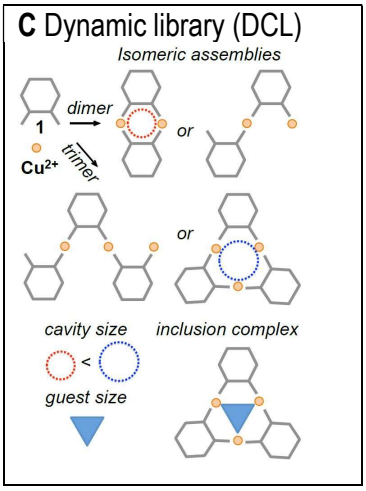


Electrospray ionization-mass spectrometry (ESI-MS) is rapid, sensitive, precise and well controlled. IMS separates **much** quicker than chromatographic techniques and is ideal for examining the size and shape of non-covalent complexes.**[1]** Together ESI-MS and IMS represent complementary methods of monitoring target solutions on a millisecond timescale. **It would be great to work with students on the following projects this year:**

(a) Intercepting critical intermediates from dynamic combinatorial libraries

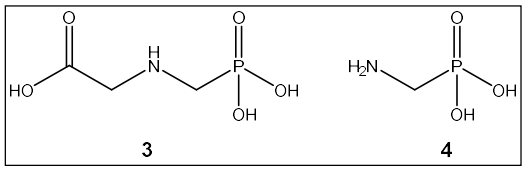
Dynamic combinatorial libraries (DCL) are mixtures of self-assembling oligomers in dynamic equilibrium (as illustrated in **C**). Depending on the angle of the ligand elbow , different shaped oligomers are feasible. Small molecules such as amines and solvents, to larger molecules like fullerenes, have been encapsulated by copper bis-β-diketonate assemblies. This makes them ideal targets for gas encapsulation, where specific cavity sizes can be prepared for target gases (e.g. CO_2).

In this project robotically controlled nESI-MS will be used to measure the stoichiometry of evolving molecular assemblies, formed from DCLs.



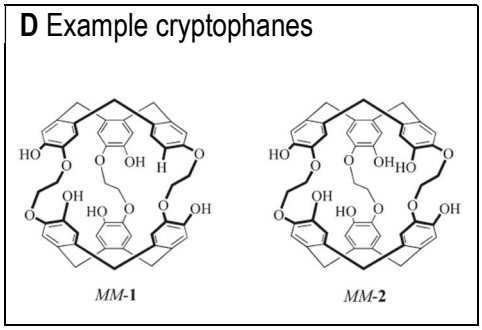
(b) Complexes of Glyphosate and Aminomethylphosphonic acid by combinatorial MS

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



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

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



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

(d) Metal – ligand clusters as model systems for enzymatic sites at the molecular level

The ability to control chemical reactions is determined by the ability to observe them, this is no less true for enzymatic reactions or reactions involving self-assembly. However, these reactions are notorious difficult to observe. In this project, advanced mass spectrometry and ion mobility will be used to study metals-ligand assemblies of urea, guanidine, formamide and nucleobases in the gas phase. These serve as a well-defined model system for enzymatic sites at the molecular level.

[1] O. H. Lloyd Williams and N. J. Rijs, Front. Chem., 2021, 9 DOI:10.3389/fchem.2021.682743.

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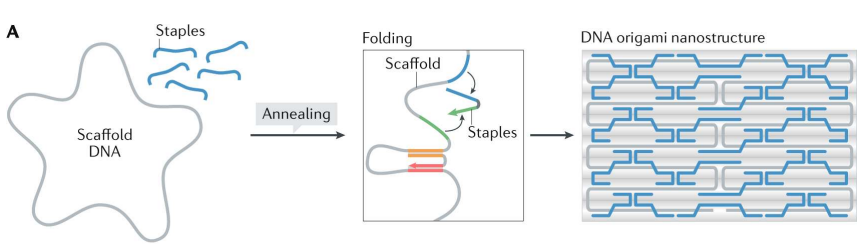
DNA NANOTECHNOLOGY AND SELF-ASSEMBLY

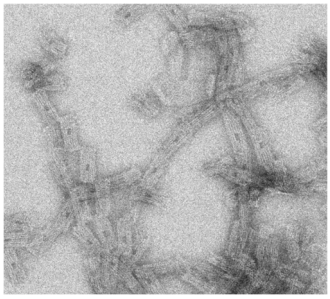
Our research looks at new ways of synthesising and manipulating soft materials built from DNA and RNA. We take nucleic acids out of their biological context and use them to construct 'Lego' building blocks and nanorobots for sensing, soft robotics, and replacement tissues. Our group is interested in fundamental and applied chemistry, and how we can harness chemical systems to mimic life-like processes, like self-healing, stimuli-responsiveness and, ultimately, evolution. Feel free to email me if you have any questions!

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

(a) DNA origami

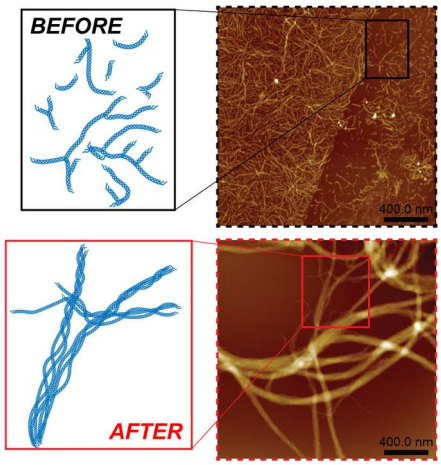
Just like you fold paper into complex shapes like swans and frogs, we can fold DNA into arbitrary geometries, like the bricks shown on the right below. We do this by adding several hundred 'staples' to a large 'scaffold' strand. We are interested in new methods to control this process, and ways in which 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) Making 'perfect' nanomaterials

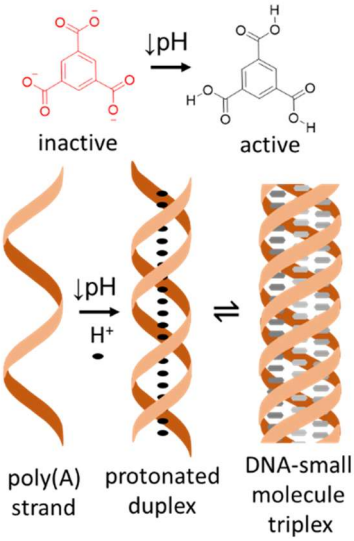
No material is perfect – even the most robust can have defects, cracks, and scars at the nanoscale. We can tune the energy landscape of materials assembly by 'pushing' these structures away from their equilibrium positions. As these systems relax to their energy minima, components are released slowly, healing defects and producing more structured, higher-performance nanomaterials. In this project we will develop new pathways for using chemical fuels and light-activated switches that rip nanomaterials apart. Instead of simply heating up and cooling down, we will develop new methods using chemical energy to direct the formation of



functional nanomaterials. A sample of what we can currently do is shown to the right – using this technology we can modulate the properties of biopolymers – including DNA and peptides – converting highly interwoven materials (before) into nanocable superstructures (right).

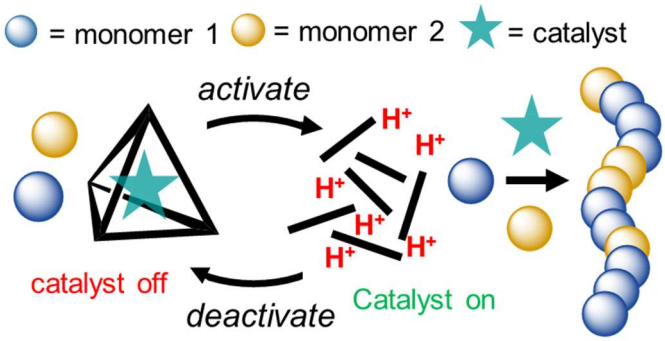
(c) Building self-assembled polymers with DNA

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.



(d) Catalytic modulation using chemical systems

Inspired by nature, we are interested in developing new modes of regulating catalysis using a 'catch and release' protocol – molecules are sequestered into high energy states, modulating their concentration upon release. This project uses chemical fuels to regulate catalytic activity and develop new classes of polymer materials. We are interested in exploring a range of structures with interior cavities capable of storing molecules: these molecules act as 'cages' that house active components until they are released.



Students in my group will also have the opportunity to collaborate with labs in England and Canada, as well as other labs in Chemistry 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

Relevant publications: ***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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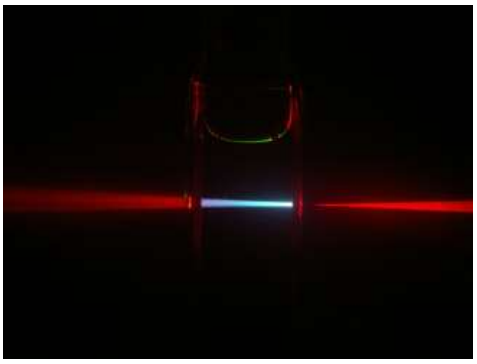
ELECTRONIC PROCESSES IN MOLECULES

My research group investigates how molecules interact with light, and the consequences, with applications ranging from studying radicals and ions of astrophysical and atmospheric interest, to renewable energy. Our principal tools are femtosecond and nanosecond lasers, with sophisticated detection schemes, vacuum chambers and mass spectrometers. We also like to do quantum theory.

ARC Centre of Excellence in Exciton Science

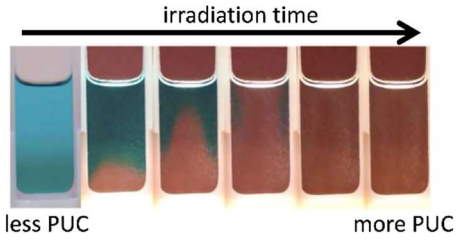
Molecular excited states within a solid can migrate. We call that mobile excitation an “exciton”. In the ARC CoE in Exciton Science, we study how to use excitons to bring about a sustainable energy future.

(a) Solid-State Upconversion Materials for Improved Solar Energy Conversion (with Dr Feng)



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

To create new devices with upconversion, including solar cells and light emitting diodes, it is important to control the triplet-triplet interactions in the solid state. In this project, we will engineer new materials with finely tuned electronic interactions to turn infrared into visible light.



(b) Molecular Switches in Upconversion (with A/Prof. Beves + Dr Alves)

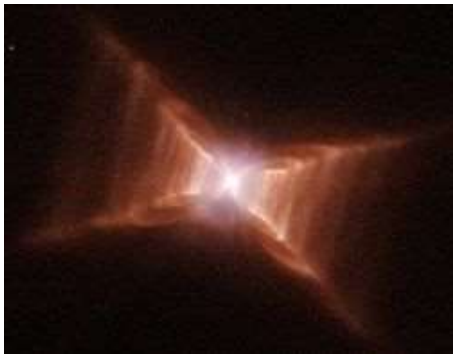
To better understand and tune upconversion, we can incorporate molecular switches. Those molecules can reversibly change their physical and chemical properties upon light irradiation of a particular colour. By linking molecular switches with molecules able to undergo upconversion, the photoswitches may inhibit or favour upconversion. Such experiments could help elucidate the effect of the spatial arrangement and be of guidance on the design of future systems. Controlling upconversion also has applications in 3D laser lithography as we can use the same concept to control the crosslinking in a photoresist.

In this project, we will design molecules for upconversion bonded with photoswitches and investigate their upconversion efficiency upon different stimuli.

(c) Laser Spectroscopy of Isolated Radicals and Ions (with Dr Chris Hansen)

The new *Molecular Photonics Laboratory* houses sophisticated lasers and equipment with which we can discover new transient chemical species of importance in the gas phase chemistries of our atmosphere and the interstellar medium.

Interstellar Molecules and Ions



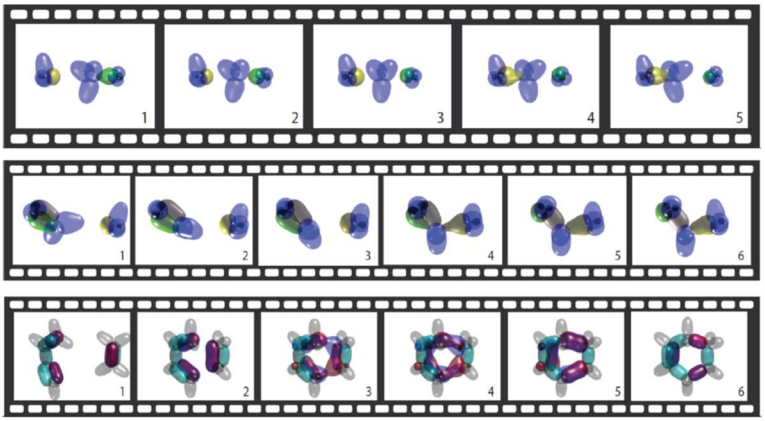
As stars die, they eject complex organic molecules into the interstellar medium, where they live out millennia before being incorporated into new stars and planetary systems. These organic molecules are the seeds of life, but, as yet, we do not know the chemical make up of the interstellar medium from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

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

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

(d) Molecular Electronic Structure – a Pan-Dimensional Approach

The electronic wave function of molecules is highly dimensional. Even water, a small molecule, has a 30-dimensional electronic wave function. How can we, as 3-dimensional beings inspect the answers of sophisticated quantum chemical calculations? We have figure out a trick. The wave function has a property known as antisymmetry: If the coordinates of two electrons of the same spin are swapped, the wavefunction changes sign, but not magnitude. This means the wave function is "tiled" in the 3*N* dimensional space. We have developed ways to calculate the structure of this tile, revealing that within the calculated wavefunction lies many motifs held close to the heart of chemists: e.g. Lewis structures, curly arrows. This project is only just getting warmed up, but has so far generated worldwide interest.



If you like coding, and quantum theory, this could be the project for you!

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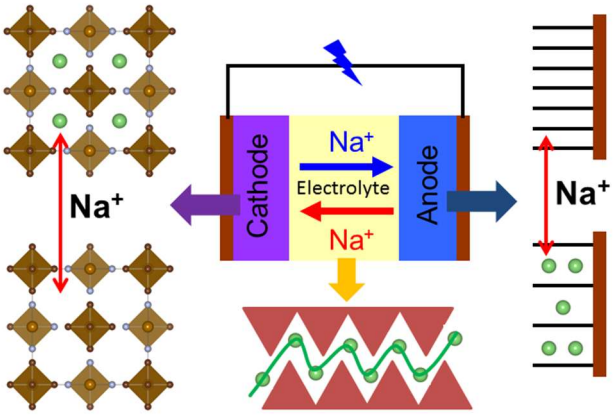
SOLID STATE AND MATERIALS CHEMISTRY

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

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

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

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



Positive electrode materials

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

Electrolytes

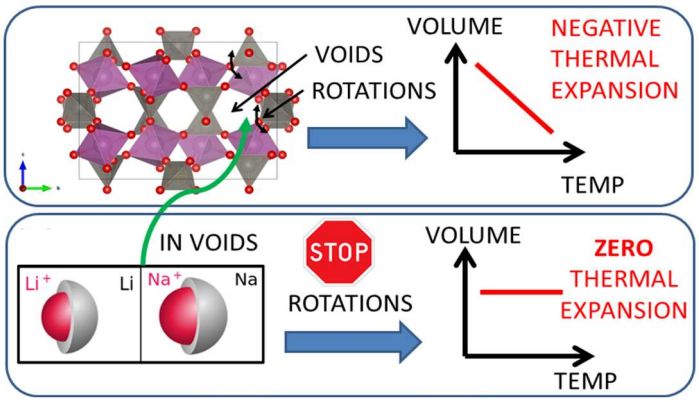
Sodium-ion conducting ceramics or glassy-ceramics are known to be excellent electrolytes at high temperatures (>300°C). This project works towards making materials with sufficient sodium-ion conduction at room temperature.

Negative electrode materials

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

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

The majority of materials expand during heating *via* thermal expansion and this process is responsible for billions of dollars per year in maintenance, re-manufacture and replacement costs due to wear and tear on both moving parts (*e.g.* in aircraft gas turbines), and components that are designed to be static (*e.g.* in optics, coatings, electronics). If a zero thermal expansion (ZTE) material can be made, a material that neither expands nor contracts upon heating, this could dramatically reduce industrial costs. In order to achieve this, the opposite extreme of materials are considered in this project - negative thermal expansion (NTE) is a property exhibited by a small group of materials predominantly due to transverse vibrations of atom groups or cooperative rotations of units (*e.g.* –CN- or WO_6). These materials typically feature large crystallographic voids and cations with variable oxidation states. So why not use a battery as a synthesis tool? In this project we will controllably insert Li and Na into the voids of the NTE materials, via a battery, in order to tune the cooperative rotations to produce ZTE materials.



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

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

(d) Other projects

Depending on your interests, other solid state projects, *e.g.* making new superconductors, can be designed. Please consult with Neeraj for further details.

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NANOPARTICLES AND TAILORED POLYMERS FOR CANCER TREATMENT

In our group, we are interested in making new polymers and nanoparticles. These nanoparticles are used to enhance the delivery of drugs for the treatment of cancer or infections. While we mainly work on the interface to biology, we can use our polymer synthesis knowledge to tackle other problems.

It would be great to work with CHEM3998/2008 students on the following projects:

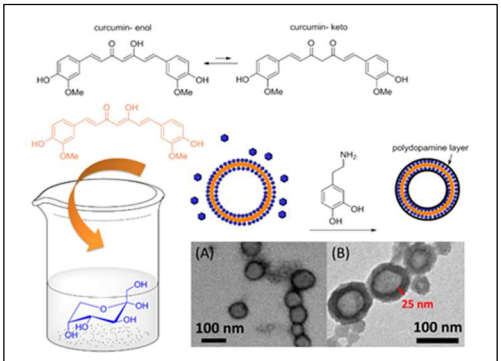
(a) Making polymers

Traditionally, polymers are made by using a solution of monomers, adding an initiator, and heating the solution. We work on other techniques that can make polymers, which can include light or a hammer. It is well-known that light can initiate polymerizations, which can be used make patterns in the material. This is for example used in 3D printing photolithography. Our group has also discovered that we can use mechanical impact to start a polymerization, basically with the impact of a hammer.

In this project you would use new forces to make polymers. You would learn to run polymerizations, but also test the materials.

(b) Nanocapsules

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

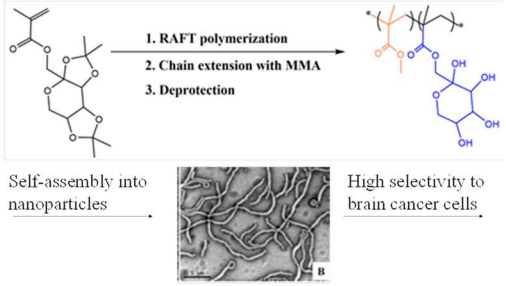


Nanocapsule by mixing of curcumin and sugars, stabilized by a polydopamine shell

In this project you would study different sugar and drug combinations and observe the stability of the solution. You would use dynamic light scattering to evaluate the size of the nanoparticles, which will be correlated to the mixture of drugs and sugars.

(c) 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 cancer.

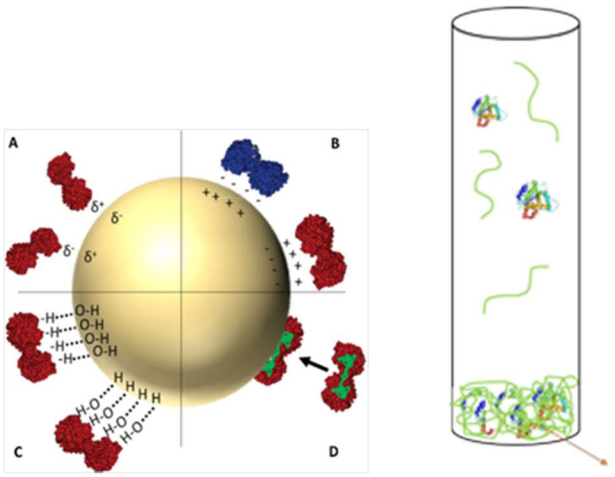


Synthesis of glycopolymers and their self-assembly into nanoparticles

In this project you would learn how to make the glycomonomer and how to polymerize it. Techniques to be used are NMR for characterization of the monomer and gel permeation chromatography (GPC) to assess the length of the polymer.

(d) Binding of polymers with protein and how we can use this

When the synthetic world (polymers, metals, ceramics) and the biological world meet the first event is that proteins, which are abundant in cells, blood and even wastewater, bind to the surface of the material. In many cases, this is an undesirable event, but sometimes it can be useful if we can target the right proteins. If nanoparticles are coated with specific proteins, they might not be more bioactive. We also use the interaction with protein to clean our waste-water. The water that enters water treatment plants is full of organic matter including proteins. Mixing this sludge water with specific polymers can bind the protein resulting in the formation of precipitating solids. The success of this process is dependent on the structure of the polymer and by optimising the polymer, we can optimise the efficiency of the protein interaction.



Interaction between polymers or polymer nanoparticles with protein is caused by the strong attractive forces, mainly electrostatic interactions, but also others (left). This can be used to trap protein from a solution to generate a polymer-protein cake

In this project you would prepare a range of polymers, which are analysed by gel permeation chromatography (GPC). After that, we will mix the polymers with various protein solutions and observe their interactions.

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MATERIALS CHEMISTRY AT THE NANOSCALE

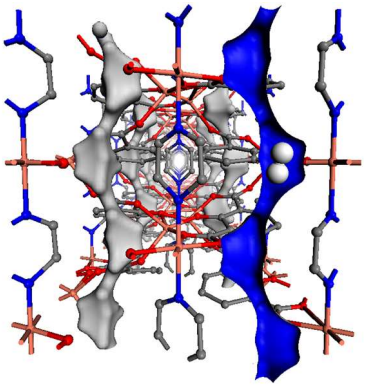
My group focuses on making and understanding new materials that are often focused on some of the major challenges facing us today: energy, water and sustainability. We make use of a range of techniques that include X-ray and neutron scattering in truly multi-disciplinary projects. Key to these studies is the notion of hierarchical emergent properties and complexity - the world around us derives from simple inter-molecular interactions; we aim for a greater understanding of these fundamental processes in order to deliver new materials displaying novel properties.

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

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

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

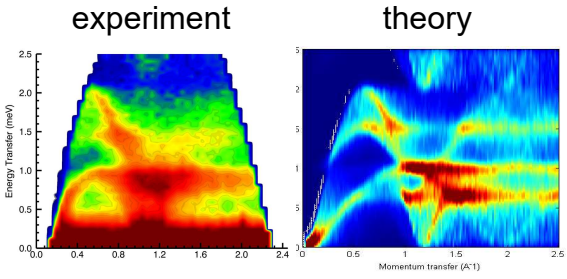
Sorting and storing molecules - how to select for one molecule over another



This research project is specifically targeted at very real challenges faced in industry - effective separations of mixed gas streams and facile storage of gaseous fuels such as H_2. Highly porous MOFs make excellent host materials for small molecules such as CH_4 or H_2. By tuning their properties MOFs can become efficient storage vessels or effective gas-selective membranes such as the H_2 selecting MOF shown here.

Quantum phenomena in magnetic materials

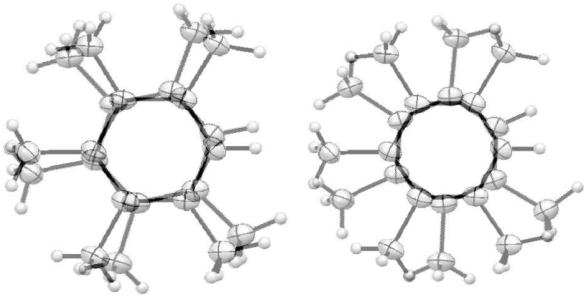
Magnetic materials have revolutionised the way in which we store and use information and have a key role to play in quantum computing; they have also been a navigational aid for centuries and are even pretty useful at securing notes to the fridge door. It is fascinating therefore that we still do not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



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

(b) Order and disorder in molecular materials

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



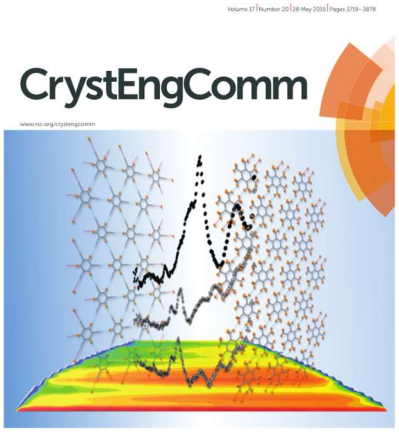
(a) crystalline phase (b) plas1c phase

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. This is where the research in the Sulway group comes in, we are exploring the synthesis and characterisation of new lanthanide containing coordination compounds that could be used in the technology of the future.

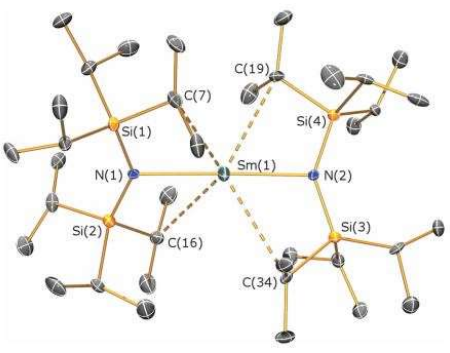
Skills you will learn:

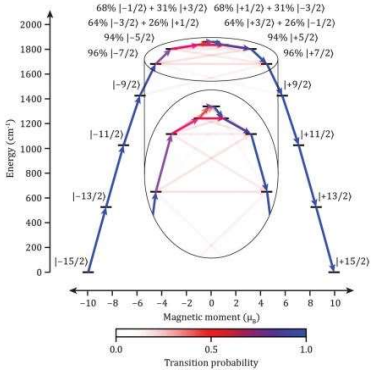
- Manipulation of air- and moisture-sensitive compounds
- Organic and Inorganic synthetic chemistry
- Structure elucidation – NMR spectroscopy (^{1}H, ^{13}C), IR spectroscopy, SQUID magnetometry and XRD (Yeap, we grow crystals)!

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

(a) Sterically hindered low-coordinate lanthanide compounds

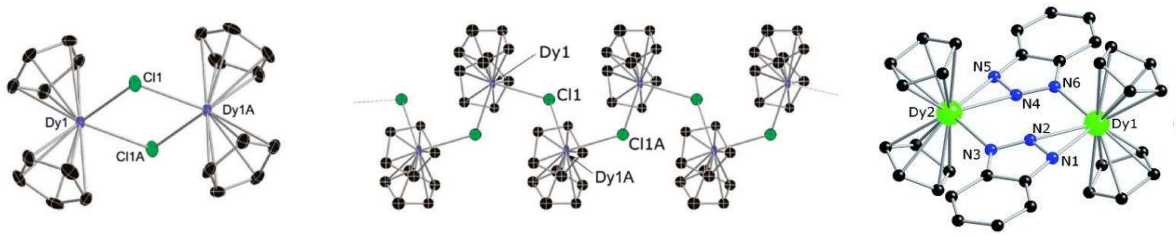
Recent insight into stabilisation of the m_J states of lanthanide containing compounds hints at the potential ability to synthesis compounds that have higher energy barriers to magnetic relaxation than any 3d-block compound. It has been suggested that even subtle changes to the coordination environment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





(b) Exploring novel linkages between lanthanide centres

As described in project (a) the smallest changes around a lanthanide centre can have dramatic changes to the magnetic behaviour of a compound. There have been a wide range of atoms used to bridge lanthanide centres but some of the more 'exotic' potential linkers are still unknown[2]… This is where you come in, this project is all about synthesising lanthanide containing compounds that have new linker molecules, we will be using a combination of 'old school' inorganic chemistry and organic chemistry to synthesis ligands that will allow us to go on and link lanthanides with such elements as P, Se and Te…



(c) Do you have an interest in education?

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

(d) Have your own ideas?

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

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

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RNA CHEMISTRY, ORIGIN OF LIFE AND NANOMEDICINE

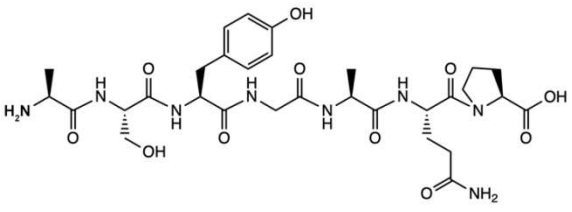
- **RNA Chemistry** with focus on understanding how RNA interacts with peptides other molecules and how these interactions can be applied in RNA science and therapeutics
- **Origin of Life and Systems Chemistry,** exploring the role of self-assembly in how life originated and how we can make life-like 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 & Dr Anna Wang School of Chemistry, Prof. Martin Van Kranendonk, BEES & A/Prof. Archa Fox, University of Western Australia).*

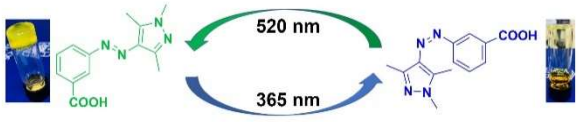
Peptides/proteins and RNA are two of the key building blocks of life. Recently it has become proteins and RNA drive the formation of lava lamp or vinaigrette "droplets"[1] within the cell but biologists are now just uncovering now how important droplet- or gel-like protein-RNA complex are in biology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

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



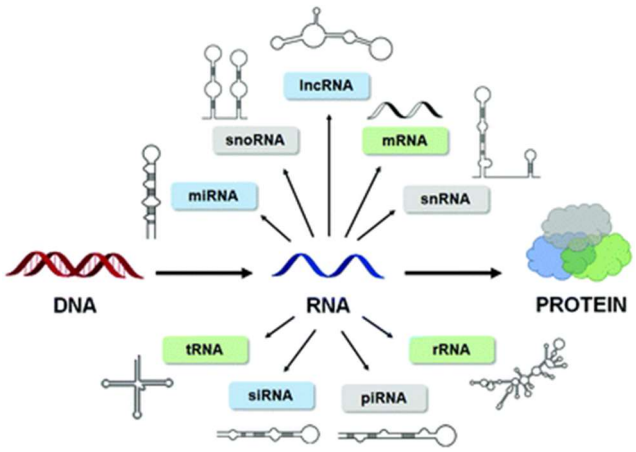
(b) Novel switchable and hybrid peptide-based materials for catalysis and 3D cell cultures *(Potential for collaborations A/Prof. Jonathon Beves, A/Prof. T. Vinh Nguyen and A/Prof. Kris Kilian, School of Chemistry).*

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, A/Prof. Joshua McCarroll 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 chemists 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.

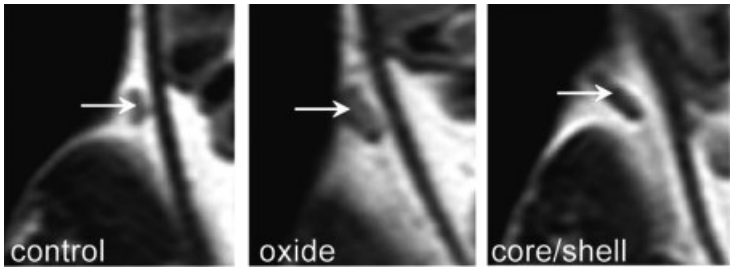

Figure 1: MRI images from iron nanoparticles injected into a mouse to enhance the contrast of a tumour.

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.

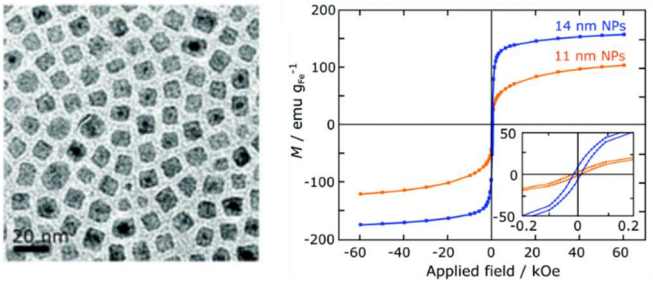

Figure 2: Transmission electron microscopy images of iron nanocubes and their magnetic properties for use in MPI.[1]

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).

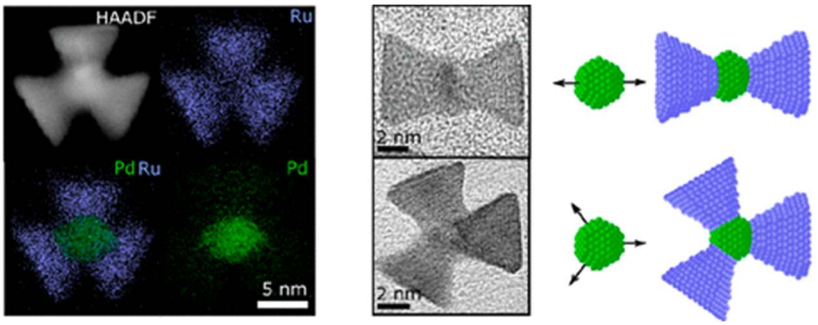

Figure 1: Energy dispersive X-ray spectroscopy elemental mapping of Pd-Ru branched nanoparticles and TEM images of individual nanoparticles. Models show the controlled direction of growth of Ru from Pd seed.

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]

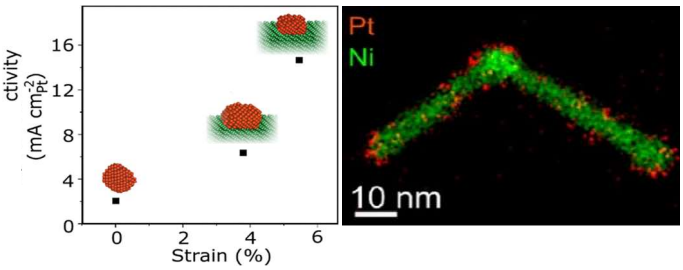

Figure 1: Relationship between strain and HER activity and elemental map of a Pt on Ni nanoparticle.[2]

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)

DR. ANNA WANG

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SOFT MATTER BIOPHYSICS AND THE ORIGINS OF LIFE

- 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 machine learning with Python.
- We have ongoing collaborations with labs in the United States, Japan, and industry.

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

(a) Building an artificial cell life cycle

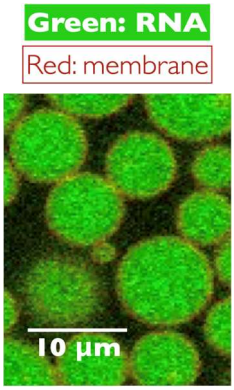

Fig. 1 Liposomes containing RNA

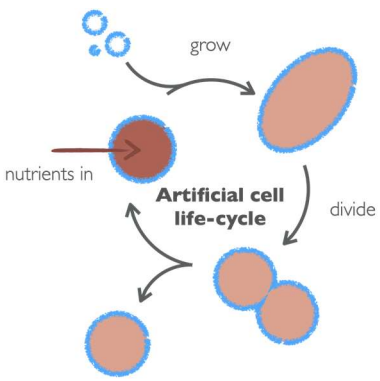

Fig. 2 A dynamic growing system

A lipid bilayer encases each of our cells (Fig 1). Lipids are also used for drug delivery e.g. mRNA vaccines, Novavax.

Being able to create a self-perpetuating artificial cell (Fig 2) reflects an unprecedented understanding of lipid bilayers, 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.

Students will learn lipid manipulation techniques, lipid vesicle/liposome processing techniques, fluorescence spectrophotometry, microscopy, and biophysics assays.
There are many sub-projects, including some as part of an international collaboration with labs in the US and Japan.

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

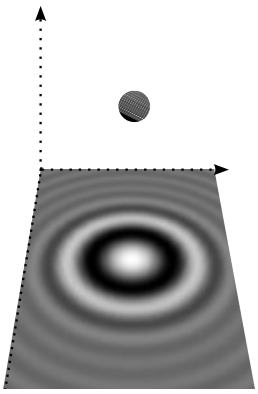

Fig. 3 Hologram of droplet

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?

To develop a mechanistic understanding, it is critical to characterise 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.

(c) 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 to solve this problem.

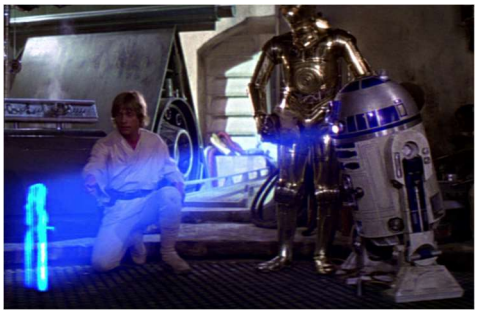

Fig. 4 "Holographic imaging" in the movies

This project 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

(d) 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.

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CHEMISTRY AND SCIENCE EDUCATION

- As part of the UNSW chemistry education group, our group focuses on learning processes, the student experience, and the role of chemistry in society. The focus is on tertiary education but is applicable to secondary education as well.
- Education research is a multidisciplinary area, and we welcome diversity for bringing new ideas and opinions! If you have a background in chemistry, science generally, or education, we would love to hear from you.
- Projects can involve engaging with other students through questionnaires or interviews (in lectures, labs, or tutorials), artifact/data collection, and/or intervention design and evaluation. We use both quantitative and qualitative analytical methods.
- We have ongoing collaborations with groups at USydney, UWA, and Curtin Uni.

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

(a) How is this test relevant? – Designing authentic chemistry assessments

(in collaboration with Dr Shannan Maisey and Dr Sara Kyne)

What sort of assessments would you like to do in a chemistry course? Will it build the skills you need for your career after university? How do you know if it is a good assessment or not? [2]

This project will use qualitative methods such as interviews and focus groups to collect data on what makes an authentic, useful chemistry assessment. Scope could include interviewing students and academics on 'ideal' assessments and core graduate skills, running focus workshops on building assessments, and analysing examples of successful assessments.

(b) I have no idea what this question means! – Metacognition in problem solving

Experts tackle problem solving almost instinctively, easily breaking down a problem to identify approaches to a solution. Novices (such as undergraduate students) are still building these skills and need the right support to do so.

How do students think about solving problems (metacognition)? Where are the sticking points and misconceptions? How can we aid in overcoming these barriers to build problem-solving skills?

This project could cover any tricky problems you've come across in chemistry. Some ideas are how we interpret NMR spectra for compound identification[3], how we design synthetic pathways, and how we

[2] Madeleine Schultz, Karen Young, Tiffany K. Gunning & Michelle L. Harvey (2022) Defining and measuring authentic assessment: a case study in the context of tertiary science, Assessment & Evaluation in Higher Education, 47:1, 77-94, DOI: 10.1080/02602938.2021.1887811

propose mechanisms[4]. Focusing on metacognition, this project would use assessment analysis to capture common misconceptions and 'think aloud' interviews to track students' thinking processes.

(c) Creativity in Chemistry – thinking outside the conical flask…

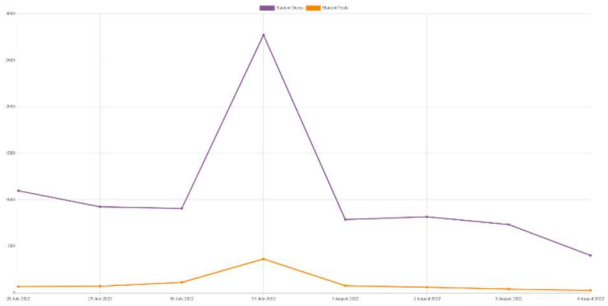
Chemistry can seem like an endless cycle of learning theories, but being a chemist is all about being able to think *big and creatively* – using innovative chemistry to solve wicked problems (just look at all the ideas in this book).

What does creativity in chemistry look like? Areas that others have explored range from "What does an atom sound like?" and science in the pub, to dance your PhD.

In this project we are interested in investigating how to bring creativity into the undergraduate classroom and what affect it has on learning and enjoyment of chemistry.[5]

The methodology of this project would be defined by what area of creativity you would like to investigate. One subproject in collaboration with Dr Laura McKemmish is writing creative chemistry questions, but there are many other areas we can look at ranging from learning activities to lab experiments.

(d) Learning analytics and student engagement



(in collaboration with Dr Sara Kyne)

How engaged do you feel in your courses? What can be done to increase this engagement to benefit learning?

This project would focus on the collection and analysis of anonymous learner data from online modes only. This would be a quantitative project using a range of statistical tests to investigate the relationship between online engagement and term timeline, course coordinator contact, resource availability, and assessments. This could be coupled with an engagement intervention such as specifically timed course coordinator emails or release of a learning resource and the effect on overall engagement or assessment performance could be measured.

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

We are keen to explore all aspects of science education and learning, and this means there are endless possible projects. If you have any curious questions you want to explore, speak to Siobhán to see what's possible.

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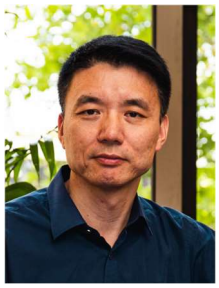
[3] Connor, M. C.; Finkenstaedt-Quinn, S. A.; Shultz, G. V., Constraints on organic chemistry students' reasoning during IR and 1H NMR spectral interpretation. Chemistry Education Research and Practice 2019, 20 (3), 522-541.

[4] Caspari, I.; Kranz, D.; Graulich, N., Resolving the complexity of organic chemistry students' reasoning through the lens of a mechanistic framework. Chemistry Education Research and Practice 2018, 19 (4), 1117-1141.

[5] Rees, S.; Newton, D., *Creative Chemists: Strategies for Teaching and Learning*. CPI Group: U.K., 2020.



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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.

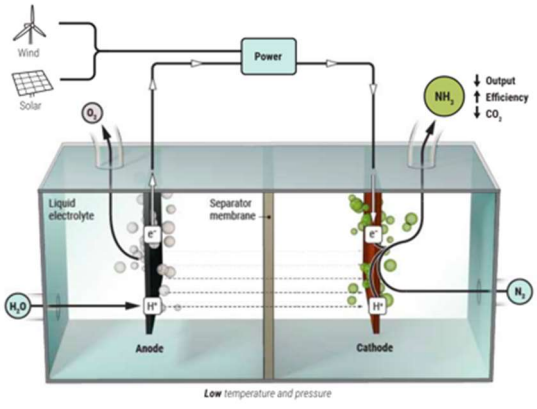
It would be great to work with Honours students on the following projects:

(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**

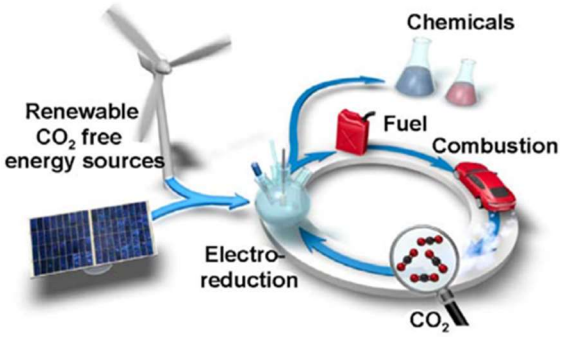
Ammonia (NH_3) is one of the most important and widely produced chemicals worldwide for fertiliser production and is also a promising liquid hydrogen carrier to be used as a carbon-free fuel. N_2 has a very strong triple bond and is extremely inert. Currently, the synthesis of NH3 is still dominated 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.