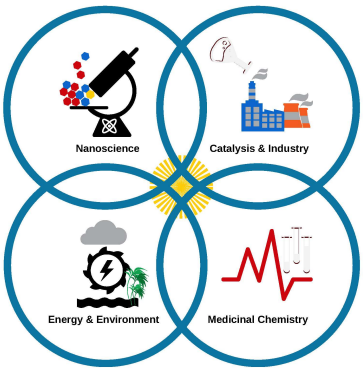
UNSW AUSTRALIA

Never Stand Still | Science | School of Chemistry

CHEM2999 & CHEM3998 Research Projects in Chemistry 2022

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.

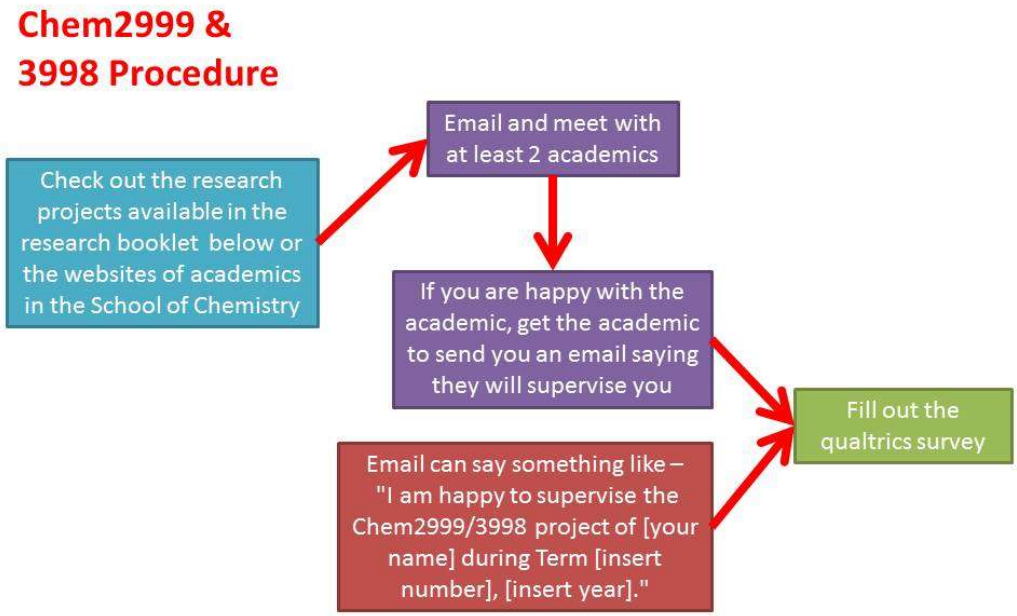
THE ENROLMENT PROCEDURE

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

Level 1, Dalton Building (F12)

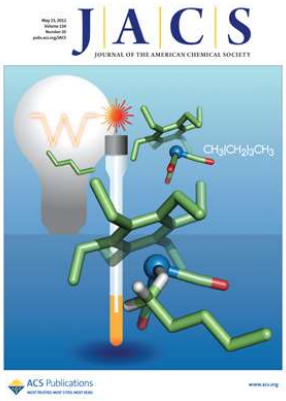
T: 9385 4720 E: g.ball@unsw.edu.au

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

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

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

(a) Short-lived metal complexes and reactive intermediates

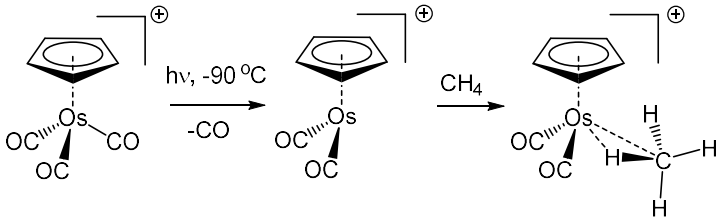


We use photochemistry in combination with *in situ* NMR at low temperatures to study molecules that have fleeting existence at room temperature. With this strategy, we have observed several types of alkane complex[1,2,3] including the *JACS* cover opposite[1] and even complexes where xenon acts as a 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.



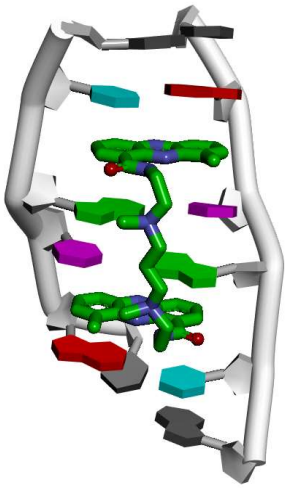
(ii) Computational design of new exotic molecules: alkane and noble gas complexes

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)

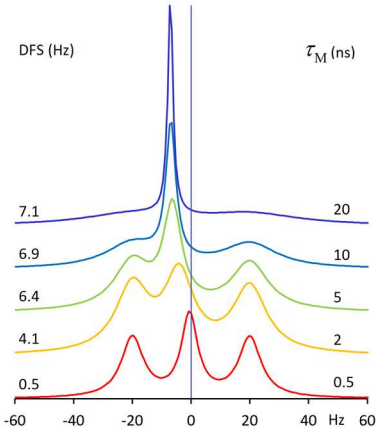


DNA presents one of the most logical and practical targets for anti-cancer therapeutics. We are investigating the binding of several mono and bis-intercalating molecules that show promise as next generation anti-cancer drugs and also the binding of clinically established drugs such as mitoxantone. The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

A/PROF. JON BEVES

Level 2, Dalton Building (F12)

T: 9385 4673 E: j.beves@unsw.edu.au

SUPRAMOLECULAR AND COORDINATION CHEMISTRY

- Supramolecular Chemistry
- Coordination Chemistry
- Molecular Machines

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

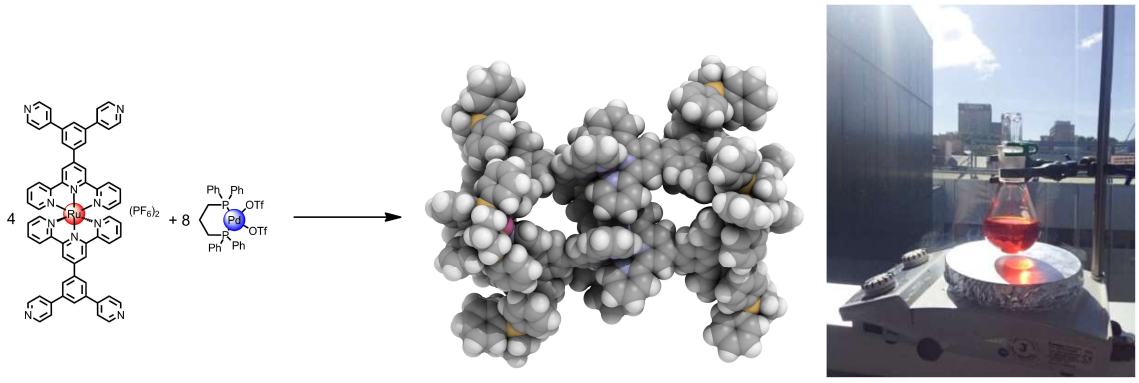
It would be great to work with Honours students on the following projects:

(a) Photoactive molecular cages

(in collaboration with Dr Evan Moore, UQ)

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

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



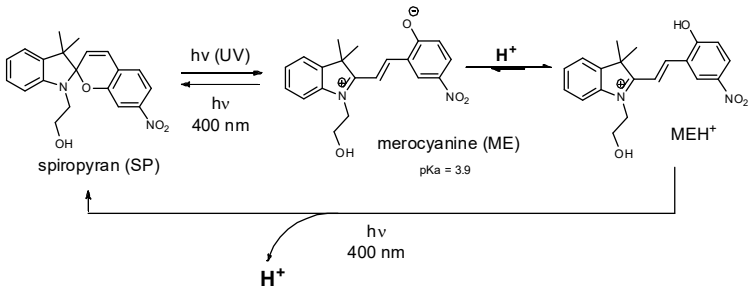
(b) Photoswitchable molecules

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

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

ON/OFF catalytic activities. One example are spiropyran molecules, which act as 'photoacids', being switched between stable acidic and non-acidic states using light stimulus. Photoacids based on spriopyran may be directly incorporated into molecular and supramolecular systems for applications in stimulus-responsible switching with applications ranging from synthetic catalysis to *in-situ* drug release. New photoacidic molecules are required which are suitable for building into larger structures and membranes, and the tuning their photoswitching properties will be studied using a combination of spectroscopic techniques.

Skills: organic synthesis, multidimensional NMR spectrometry, mass spectrometry



(c) Novel ruthenium(II) complexes

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

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

(d) Molecular rotors

(in collaboration with A/Prof. Jason Harper)

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

Skills: Organic synthesis, multidimensional NMR spectrometry

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

1. *Yang, J.; Bhadbhade, M.; Donald, W. A.; Iranmanesh, H.; Moore, E. G.; Yan, H.; Beves, J. E. Chem. Commun.* ***2015****, 51, 4465-4468.*

A/PROF. ALEX DONALD

Level 6, SEB Building (E8)

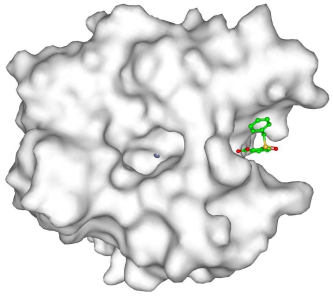
T: 9385 8827 E: w.donald@unsw.edu.au

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.

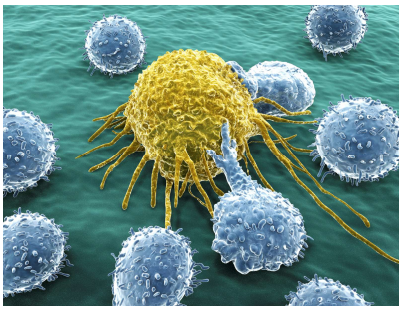


Where does the drug bind? Methods for rapidly pinpointing where small molecules bind to druggable targets are urgently needed for discovering the next generation classes of bioactive molecules.

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. ALBERT C. FAHRENBACH

Level 7, Hilmer (E10), 719

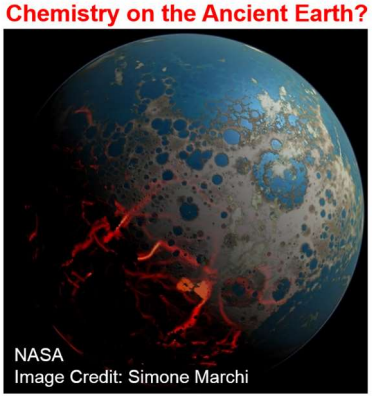
E: a.fahrenbach@unsw.edu.au

W: fahrenbachresearch.com

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?

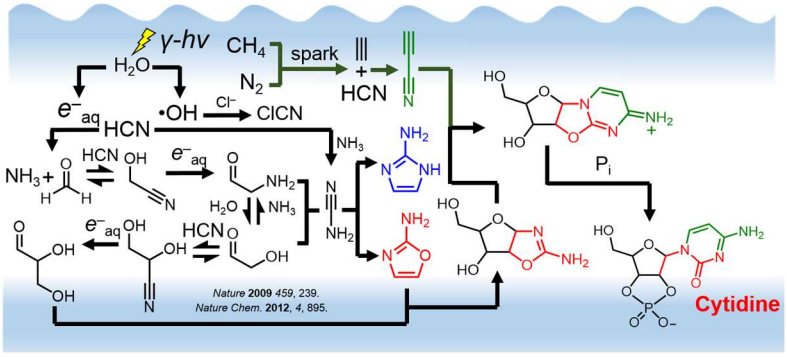


I am a new Lecturer starting in the School of Chemistry ready to take on students. Students may have potential opportunities to collaborate with and visit scientists from NASA Astrobiology labs in the US, as well as researchers from the Earth-Life Science Institute at the Tokyo Institute of Technology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

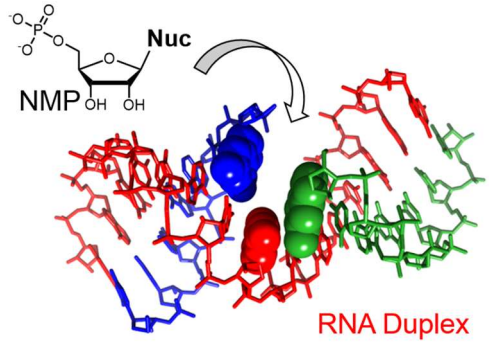
The need to make, measure and model complex reaction networks, especially those that give rise to hypothetically relevant prebiological compounds like ribonucleotides and amino acids, is fundamentally important for addressing the chemical mysteries shrouding life's origins. The goal of this project is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

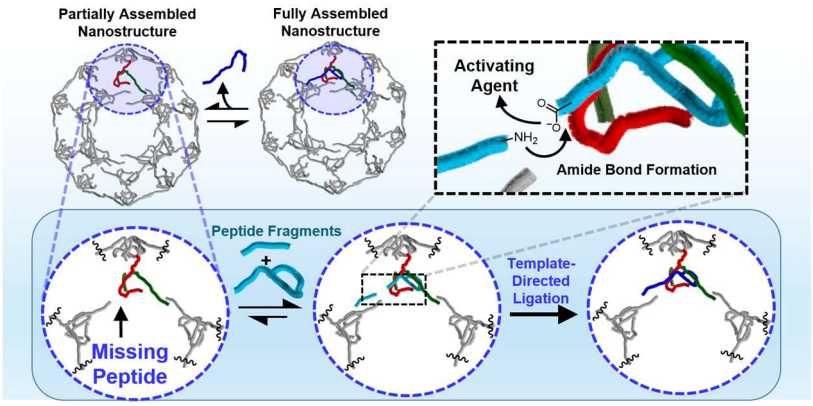


RNA is often hypothesized to be among the first genetic polymers to have arisen abiotically from chemical evolution on the early Earth. The template-directed replication of RNA – without the aid of modern enzymes – offers a mechanism by which Darwinian evolution may have originally initiated. The objective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

PROF. LES FIELD

Room 1009, Level 10, Chemical Sciences Building (F10)

E: L.Field@unsw.edu.au

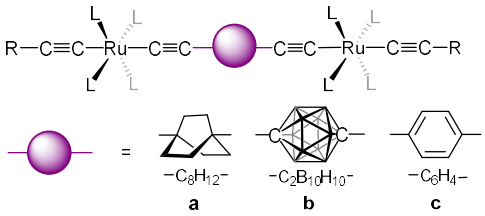
SYNTHETIC ORGANOMETALLIC CHEMISTRY

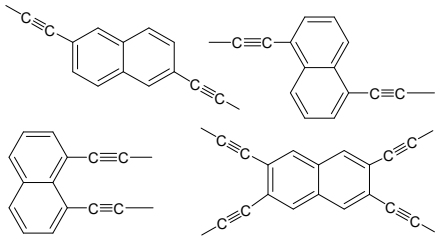
- Research in the Field group is centred around synthetic organometallic chemistry:
  - Development of organometallic catalysts that are able to activate small molecules (such as N_2, CO_2, CH_4 *etc*), and to functionalise organic hydrocarbons (CH_4, ethylene, acetylene *etc*) to make value-added products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



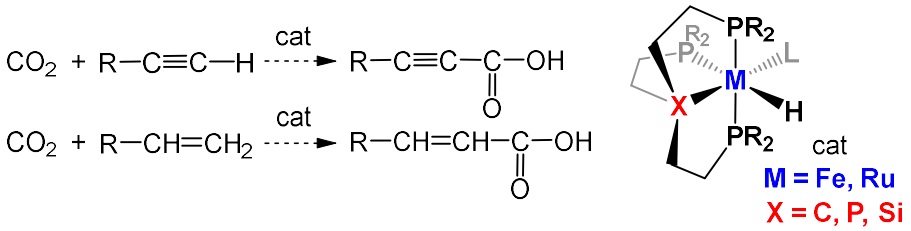


The majority of alkyne-bridged organometallic polymers use linear aromatic spacer units as the bridge between metal centres. We are interested in introducing bridges based on naphthalenes and other aromatic systems as well extending the oligomers to 2- and 3-dimensional networks.

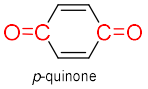
(b) The Organometallic Chemistry of Carbon Dioxide

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.

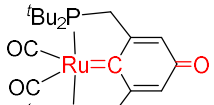


(c) Metal-to-metal communication through cross-conjugated frameworks (with Dr Martin Peeks)

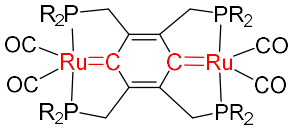


p-quinone

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.



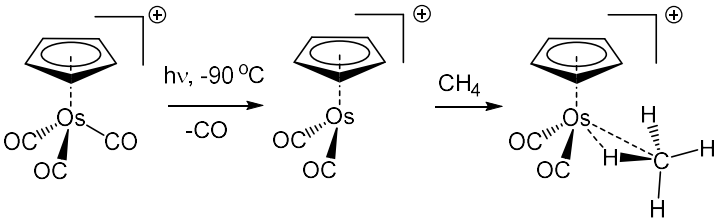
metallaquinone



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.

SCIENTIA PROF. J. JUSTIN GOODING

Level 7, Hilmer Building (E10)

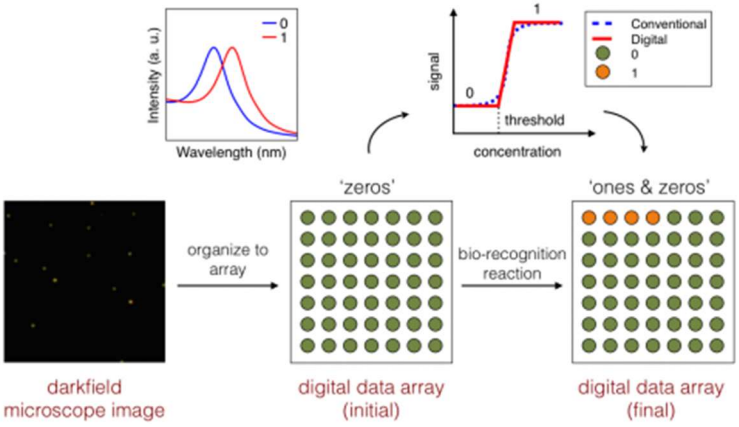
T: 9385 5384 E: justin.gooding@unsw.edu.au

Australian Centre for NanoMedicine

SMART MATERIALS AND SURFACES

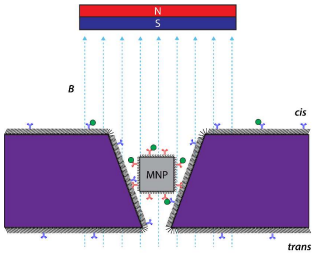
Our research group specializes in using self assembled monolayer or other surface modification technique to provide surfaces with unique functionality. The surfaces are the base upon which we build functional devices from nanscale component including polymer, protein, nanoparticles, and porous material.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

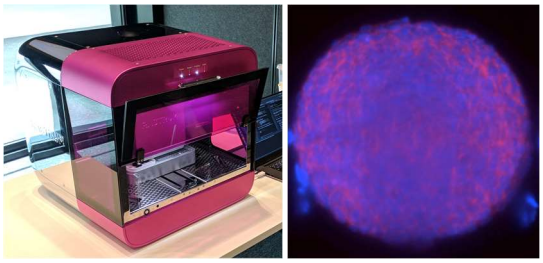


Specific antigen-antibody binding

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

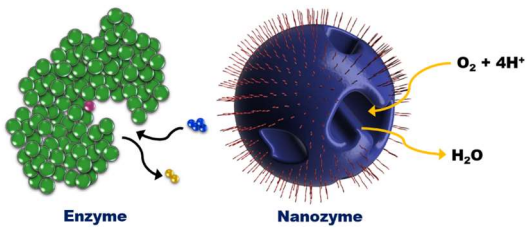
time taken for the molecules to find the nanopores. We have solved this problem by developing a new type of nanopore, referred to as a nanopore blockade sensor. In this system, antibody magnetic nanoparticles capture the analyte of interest and brign it to the nanopore. The nanopmodified nanoporesarticle 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.

Dr CHRISTOPHER HANSEN

Level 6, Science and Engineering Building (E8)

T: 9065 3085 E: christopher.hansen@unsw.edu.au

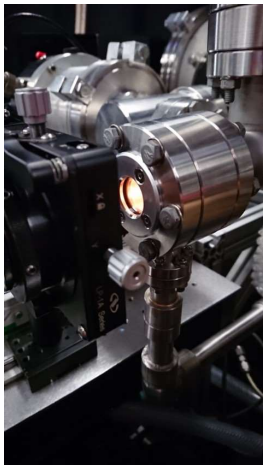
The true impact of fluorinated compounds in the atmosphere

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

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

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

(a) VUV Photodissociation of Hydrofluorocarbons



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

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

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

(b) UV Photochemistry of Hydrofluoroolefins

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

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

Recent results from my group (in collaboration with Prof. Scott Kable's group) have revealed that the decomposition product of an important next generation refrigerant (HFO-1234ze or 1,3,3,3-tetrafluoropropene), with a GWP of zero, is removed from the atmosphere via photolysis to yield a significant quantity of the worst of the HFCs *i.e.* fluoroform (CHF_3) with a global warming potential ~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.

A/PROF. JASON HARPER

Level 2, Dalton Building (F12)

T: 9385 4692 E: j.harper@unsw.edu.au

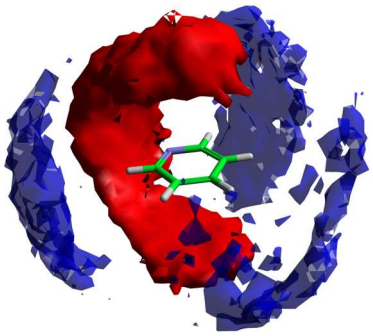
www.jasonbharper.com

MECHANISTIC AND PHYSICAL ORGANIC CHEMISTRY

Our research is focussed on understanding how organic processes happen and what affects reaction outcomes. Particularly, this work encompasses examining how structural features in both the reagents themselves and the solvent used can change how a reaction proceeds. This knowledge can then be applied to a range of fields, including bioorganic, synthetic, analytical and environmental chemistry. Being particularly interdisciplinary, there is extensive opportunity for collaboration and projects are currently underway in catalysis, reaction kinetics, synthesis and molecular dynamics simulations.

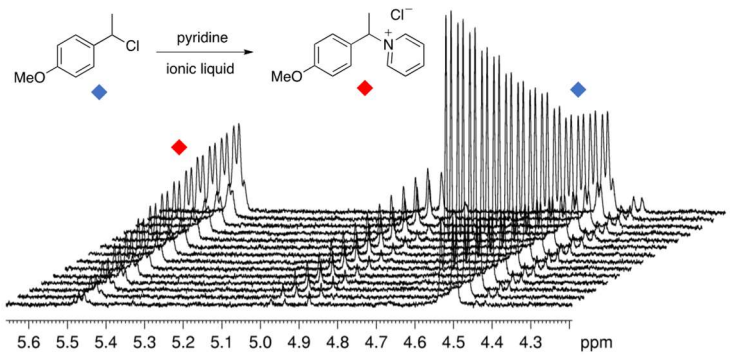
a) Ionic liquid effects on organic reactions: understanding solvation, designing better solvents and getting the reaction outcomes you want.[1] (collaborators include Dr Ron Haines & Prof. Stuart Prescott, UNSW; Prof.'s Anna Croft & Christof Jäger, University of Nottingham; Prof. Bill Price, Western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

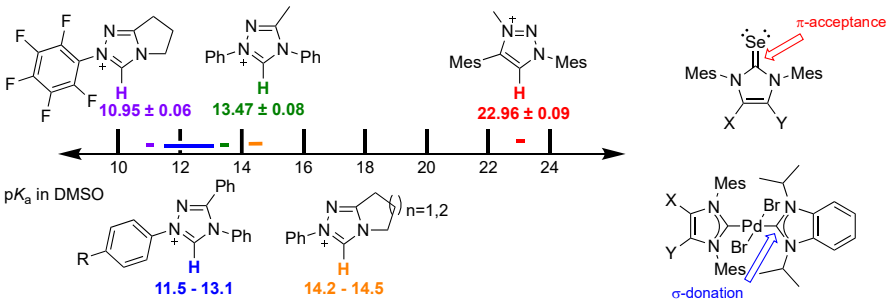
The project would involve kinetic analyses using NMR spectroscopy to monitor the progress of reactions, along with synthetic organic and analytical chemistry. Importantly, it can be readily tailored to either the physical and analytical aspects, with the opportunity to focus on methods to measure interactions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

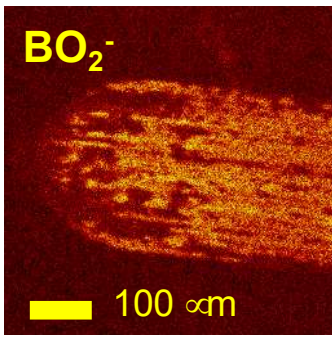
N-Heterocyclic carbenes, have significant roles in both organo- and organometallic catalysis, however some carbenes are effective for some processes but not for others; the origin of this is not well understood. This project aims to relate the structure and chemical properties of carbenes to catalytic 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 Glavitskih and Mark Rutland, KTH, Stockholm)

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



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

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

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

1. A. 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; R. R. Hawker *et al.*, *Chem. Commun.* **2018**, *54*, 2296; *Org. Biomol. Chem.* **2018**, *16*, 3453 & **2017**, *15*, 6433. For a review see *Adv. Phys. Org. Chem.* **2018**, *52*, 49.
2. C. Barnett *et al.*, *Chem. Methods.* **2021**, *1*, 374; N. Konstandaras *et al.*, *Org. Biomol. Chem.* **2020**, *18*, 66 & 1910; *ChemistrySelect*, **2017**, *2*, 718; M. H. Dunn *et al.*, *J. Org. Chem.* **2017**, *82*, 7324.
3. J. J. Black *et al.*, preprint at 10.21203/rs.3.rs-849341/v1; 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.

DR. JUNMING HO

Level 1, Dalton Building (F12), Room 126

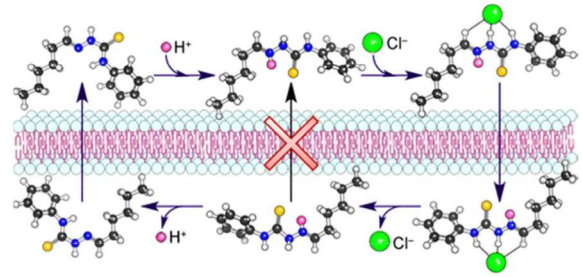
E: junming.ho@unsw.edu.au

COMPUTATIONAL CHEMISTRY AND BIOMOLECULAR SIMULATIONS

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

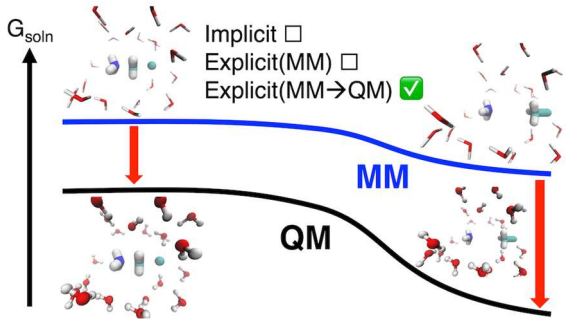
(a) Anionophores as novel anti-cancer agents

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



(b) Accurate prediction of reaction outcomes

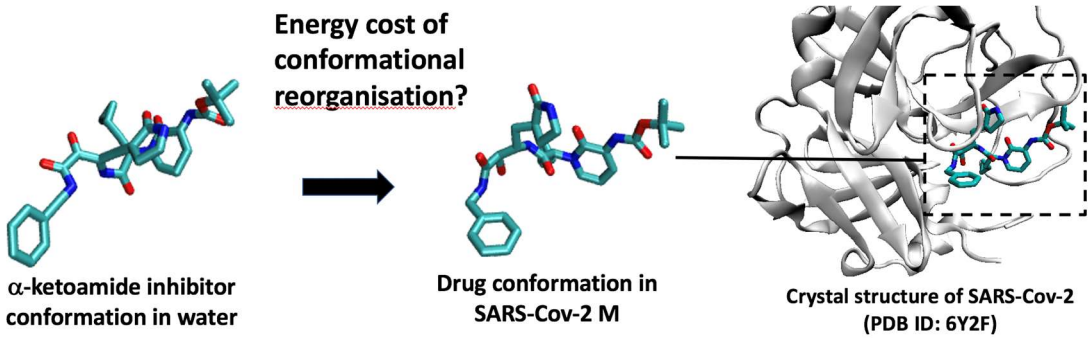
A significant milestone in computational chemistry is the development of highly accurate methods that can reliably predict the outcomes of gas phase reactions. Unfortunately, solution phase theoretical chemistry remains in a relatively primitive state where it is still very challenging to accurately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



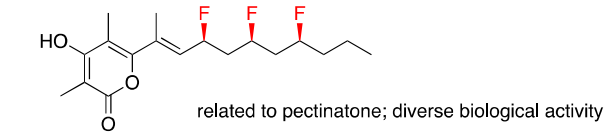
will enable chemists to reliably predict the yields and rates of chemical reactions. Specific areas include assessment of contemporary electronic structure methods to predict solvation energies and forces, and the development of efficient hybrid and fragmentation methods to accelerate their calculation.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

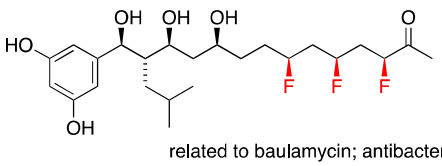
(c) SARS-CoV-2: Understanding protein-ligand binding affinity

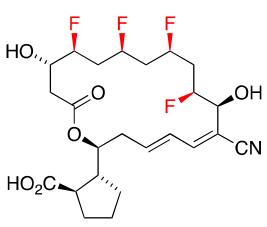
This project aims to understand how the conformational flexibility of a drug molecule may affect its binding affinity to the drug target. For example, the crystal structure of SARS-CoV-2 M^{pro} and its complex with an α-ketoamide inhibitor was recently reported (*Science* **2020**, 368, 409) and it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

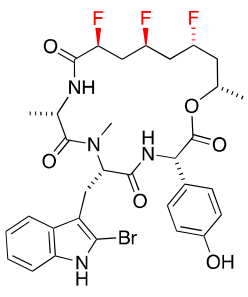


(d) Computer-aided design of fluorinated bioactive molecules (with A/Prof Luke Hunter)









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

A/PROF. LUKE HUNTER

Level 2, Dalton Building (F12)

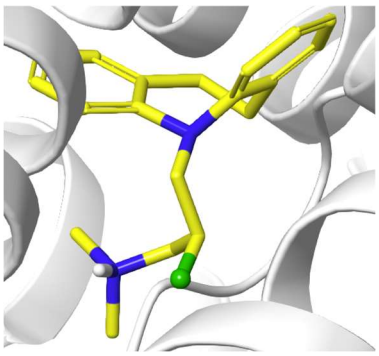
E: l.hunter@unsw.edu.au

MEDICINAL ORGANIC CHEMISTRY

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

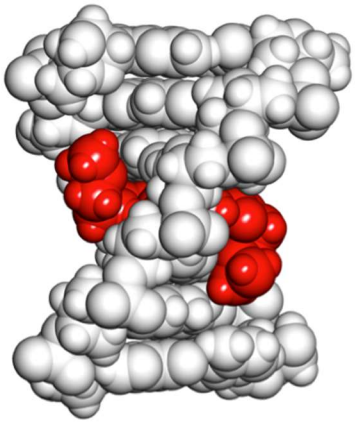
(a) "Molecular origami": using fluorine to control the shapes of bioactive molecules
(in collaboration with Dr. Junming Ho; Dr. Angela Finch [SOMS]; Dr. Nicola Smith [SOMS])

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



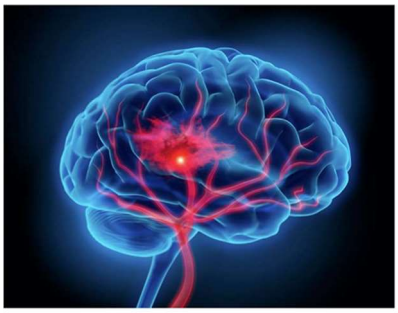
(b) "Molecular Velcro": targeting DNA to treat brain cancer
(in collaboration with A/Prof. Larry Wakelin; A/Prof. Graham Ball; Prof. Martina Stenzel; Prof. Bill Denny [Auckland]; Dr. Euphemia Leung [Auckland])

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



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

Stroke is a leading cause of death and disability in Australia, and the treatment options are extremely limited. We are pursuing a new approach. We're developing drugs that activate nerve cells' natural hypoxia protective mechanisms, which will put nerve cells into damage-control mode after a stroke.[7] The key is a molecular-level understanding of the proteins that naturally activate this hypoxia response.



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

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

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DR SINA JAMALI

Level 7, Hilmer Building (E 10), 746

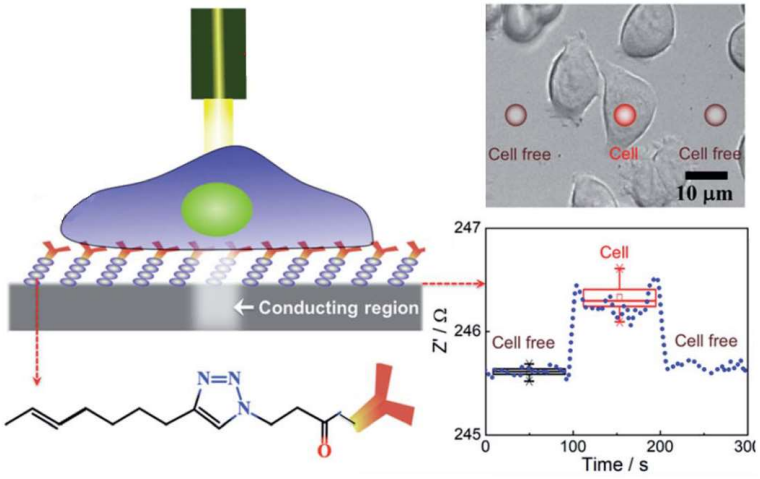
E: s.jamali@unsw.edu.au

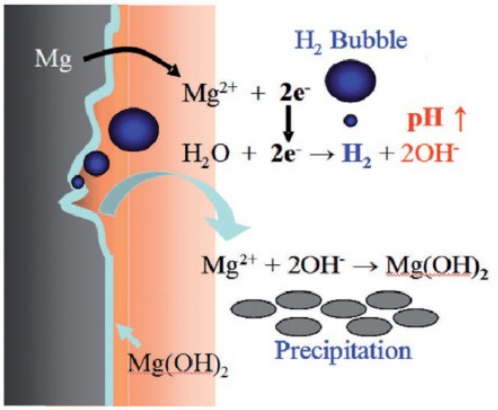
Electrochemistry of living cells and materials

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

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DR MOHIBUL KABIR

ARC DECRA Fellow

Room 722, Hilmer Building (E10)

T: 9385 1958 E: k.kabir@unsw.edu.au

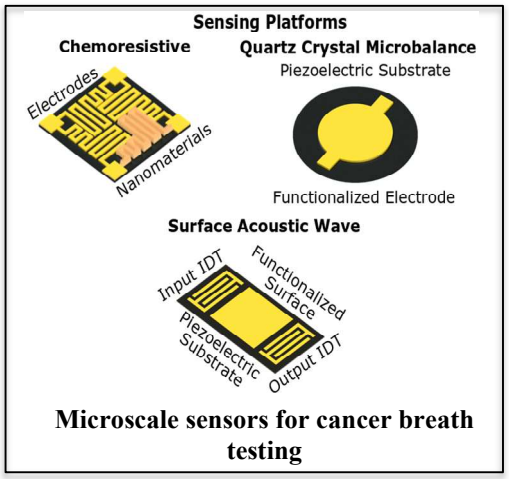
PORTABLE DEVICES FOR CHEMICAL ANALYSIS

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

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

(a) Microscale gas sensors for cancer breath testing

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



Microscale sensors for cancer breath testing

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

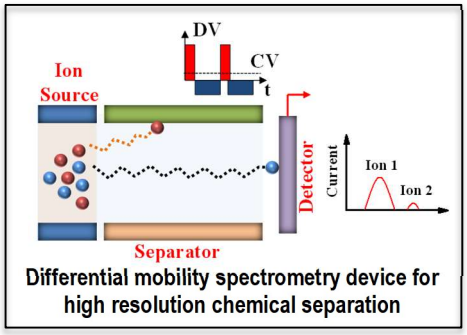
Even though commonly used gas/liquid chromatography and mass spectrometry-based methods allow universal chemical analysis with high sensitivity, they are not suitable for point-of-care diagnostics owing to their bulky size, rigorous sample pre-treatment requirement and long analysis time. Thus, recent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

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

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

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

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



Differential mobility spectrometry device for high resolution chemical separation

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

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

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

PROF. SCOTT KABLE

Level 1, Dalton Building (F12)

T: 9385 4713 E: s.kable@unsw.edu.au

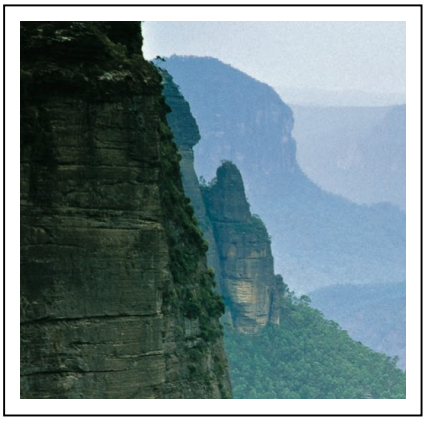
LASER PROBES OF CHEMICAL REACTIONS

- 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)

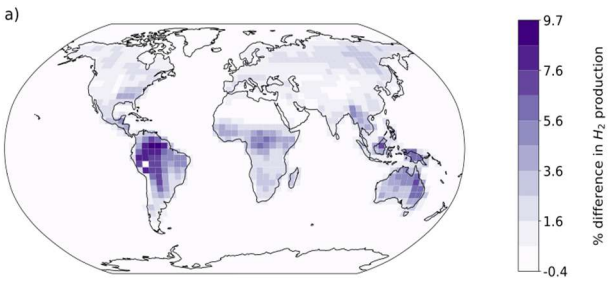


The poor state of our atmosphere is one of the most pressing issues facing society today. Everyone knows about the challenges of climate change. But did you realise that more people meet premature deaths from poor air quality than form either cancer or heart disease?

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).

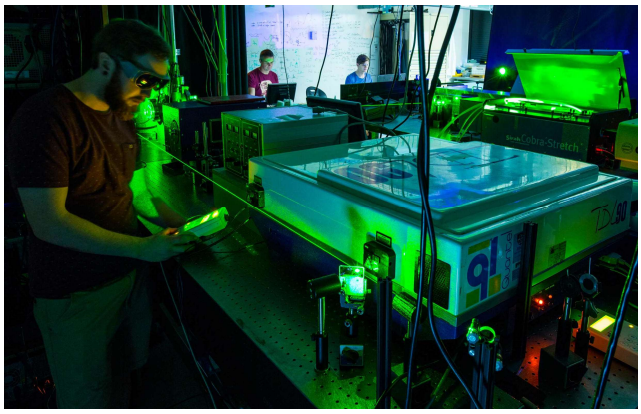


(b) Weird chemistry – reactions that just don't go where they should. (Collaborators: Meredith Jordan, Sydney U., David Osborn, Sandia National Labs, USA)

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

A/PROF. KRIS KILIAN
Level 7, Hilmer Building (E10)
T: 9385 4666 E: k.kilian@unsw.edu.au

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.

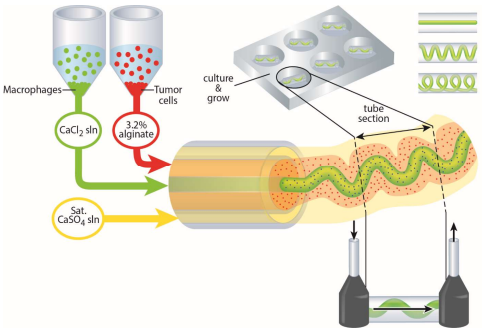


Fig. 1. Extrusion of cell-laden chemically modified alginate (*Adv. Mater., 2015*)

(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

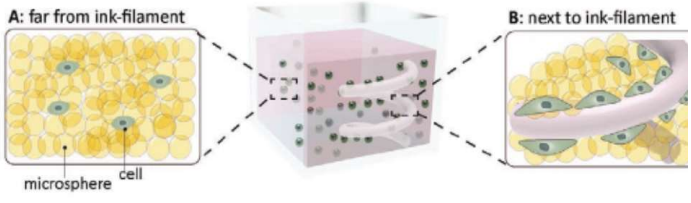


Fig. 2. Ceramic Omnidirectional Bioprinting in Cell Suspensions (Romanazzo et al., *Adv. Funct. Mater.,* 2021)

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.

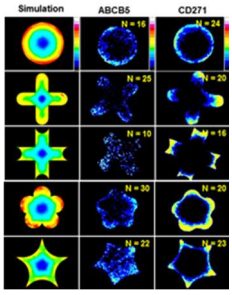


Fig. 3. Interfacial curvature will guide the activation of a stem-like state (Lee et al., *Nat. Mater.*, 2016)

(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.

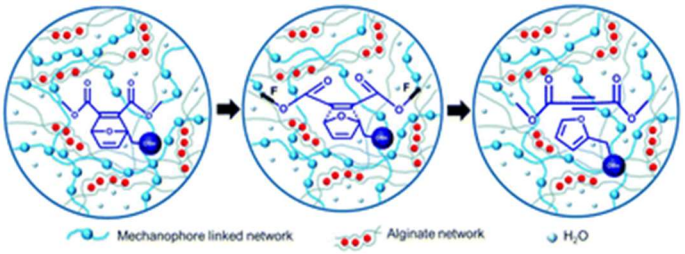


Fig. 4. Compression or tension triggers molecule release in double network hydrogels (Jayathilaka et al., Chem. Commun. 2021)

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.

DR. DONG JUN KIM

Level 7, Room 718, Science and Engineering Building (SEB, E8)

E: dongjun.kim@unsw.edu.au

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.

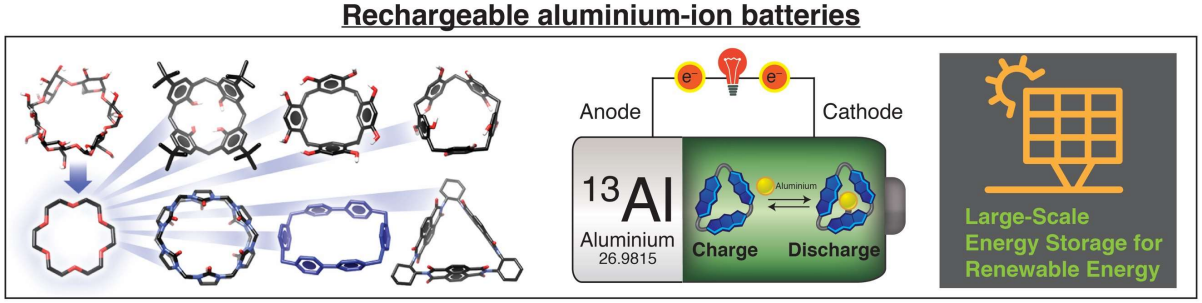


Figure 1. Graphical representation of the macrocyclic building blocks into nano-channels.

(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

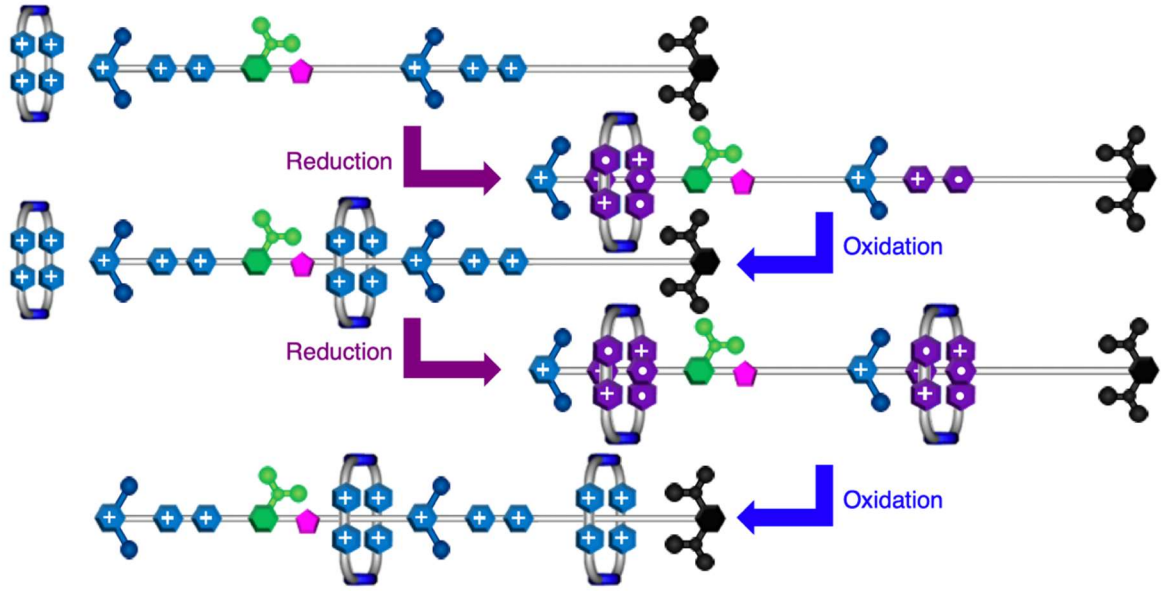


Figure 2. Structure the molecular dual pump and pumping rings onto the collecting chain chemically and electrochemically.

PROF. NARESH KUMAR

Level 7, Science and Engineering Building (E8)

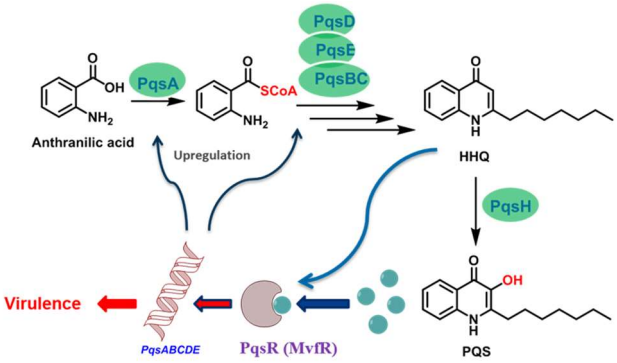
T: 9385 4698 E: n.kumar@unsw.edu.au

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.

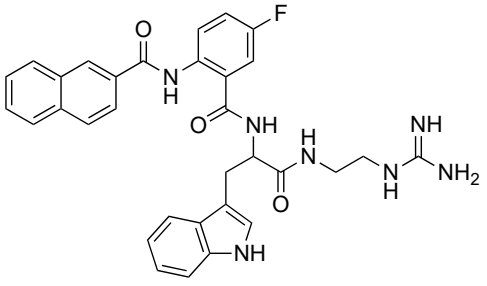
(a) DESIGN AND SYNTHESIS OF NOVEL ANTIMICROBIAL AGENTS

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.

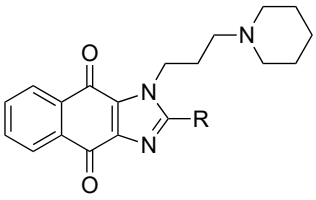
Inhibitors of Bacterial Transcription Initiation

(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.

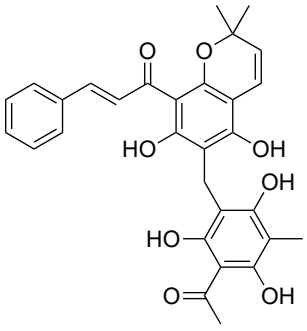
(b) DEVELOPING ANTICANCER COMPOUNDS THAT ACTIVATE GLUCOSE OXIDATION

(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.

DR. MARTINA LESSIO

Office: Room 124, Dalton Building

E: martina.lessio@unsw.edu.au

COMPUTATIONAL MATERIALS SCIENCE AND CHEMISTRY FOR SUSTAINABILITY APPLICATIONS

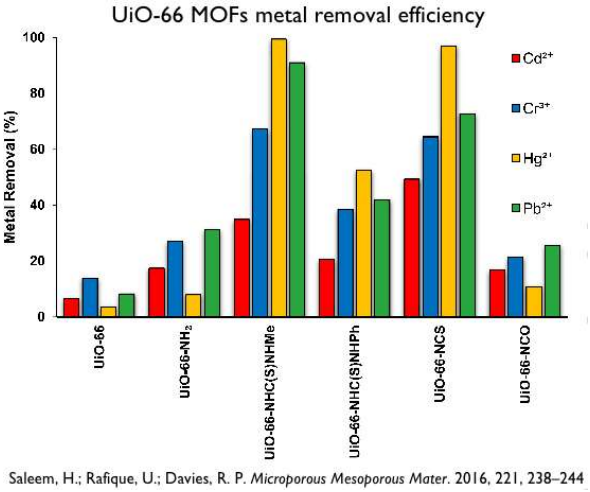
Computer simulations are an essential tool to make high-impact discoveries in fields that are crucial to our sustainable future. In general, these types of simulations allow us to calculate properties of molecules and materials at the atomic scale, which can be too difficult to be measured by experiments.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

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

Some of the projects currently available are:

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

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



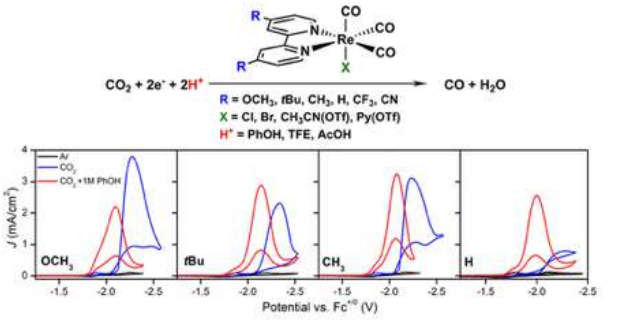
Saleem, H.; Rafique, U.; Davies, R. P. *Microporous Mesoporous Mater.* 2016, 221, 238–244

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

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

(b) Carbon Dioxide Reduction Using Transition-Metal Complexes

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



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

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

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

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

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

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

DR. SHANNAN J. MAISEY

Level 1, Dalton Building (F12)

T: 02 9385 5967 E: s.maisey@unsw.edu.au

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

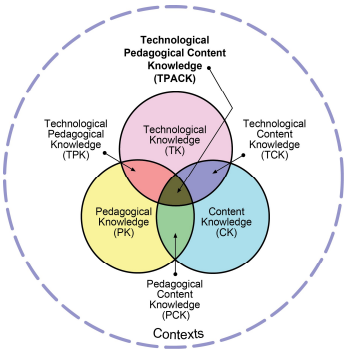
The world is currently facing unprecedented challenges which are affecting all facets of life on earth. Climate change, Sustainability and the need for Renewable energy sources and storage are challenges which have chemistry at their core. A recent article in Nature Reviews Chemistry[1] served as a call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

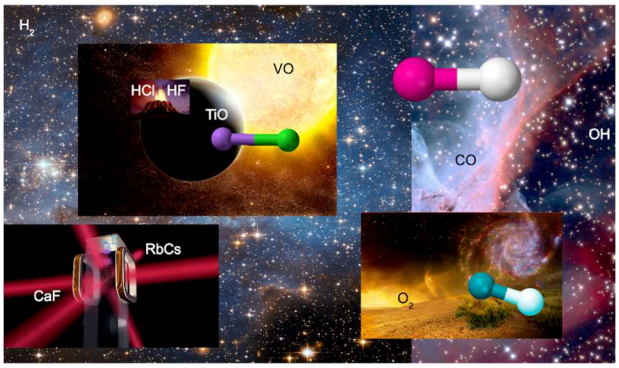


Keywords: *Digital Literacy, PCK, TPACK, Online learning, Blended Learning*

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

DR. LAURA K. McKEMMISH

Level 1, Dalton Building (F12)

E: l.mckemmish@unsw.edu.au

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

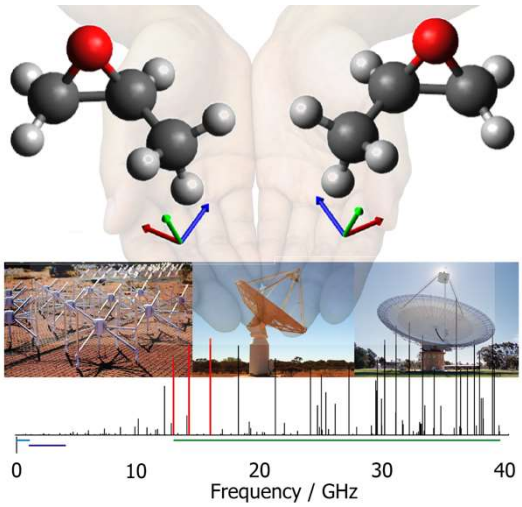
Keywords: Machine Learning, Data Science, Computational Quantum Chemistry, Supercomputers, High-throughput Calculations, Spectroscopy

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).

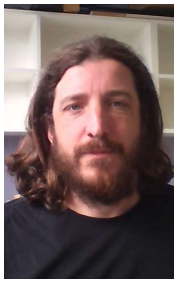
Keywords: Python, Application, Cheminformatics, Algorithm Design

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.



DR CHRIS MEDCRAFT

Level 7, Hilmer Building (E10)

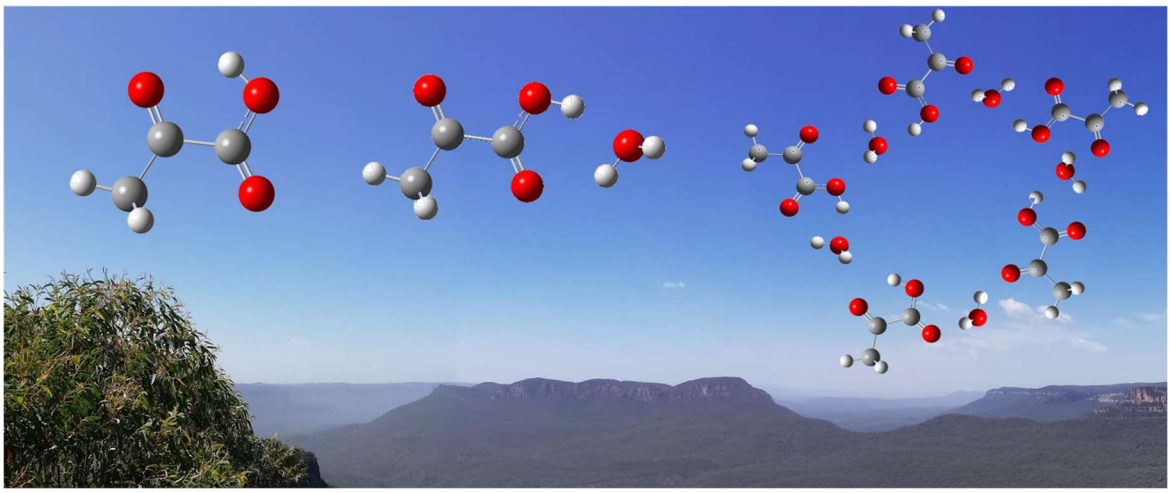
Email: c.medcraft@unsw.edu.au

PROBING ATMOSPHERIC REACTIONS WITH MICROWAVE SPECTROSCOPY

Chirped pulse Fourier Transform Microwave (CP-FTMW) Spectroscopy is a powerful new technique for rapidly acquiring rotational spectra. This allows for the precise determination of the 3D structure of gas phase molecules. I am building up the only laboratory in the southern hemisphere with such an instrument. Work in this laboratory is focused on rotational spectroscopy which involves many different skills and techniques. There will also be opportunities for experiments will to be conducted at the Australian Synchrotron at the Terahertz beamline. In addition to the recording and analysis of spectra, projects can, depending on your interests, include programming, quantum chemical calculations, instrumental development and some synthetic chemistry. The projects on offer are broadly separated into two themes: atmospheric chemistry and astrochemistry.

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

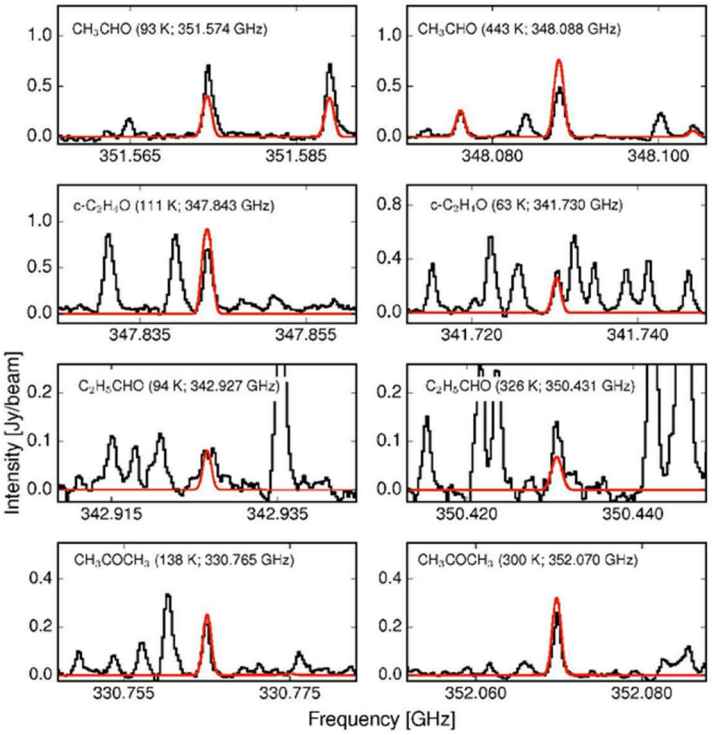
(a) Atmospheric Chemistry: examining the conformer dependence of chemical reactions in the atmosphere



Many molecules have a fine energetic balance between inter- and intra- molecular bonding that depends on the conformational landscape of the molecule. Molecular structure is inherently link to chemical reactivity, however the conformational dependence on reactivity is often overlooked. The photolysis rates of carboxylic acids in the atmosphere have been shown to have large differences between conformers. The project will develop a methodology to sample a series of small di-carbonyl and di-carboxylic acids and determine their rotational spectrum using state of the art chirped pulse Fourier transform microwave (CP-FTMW) and synchrotron FTIR spectroscopy and high-level quantum chemical calculations. The structures of monomers, dimers, and hydration complexes will be determined, and interaction energies will be estimated. By determining the conformations of the monomer units in various hydrogen bonded environments we can draw conclusions on the formation routes of larger oligomers and particle nucleation.

(b) Astrochemistry: The search for pre-biotic chemicals in space

Just over 200 molecules have been detected outside of our solar system, these are primarily found through the identification of multiple rotational absorption or emission lines from telescopes like the Parkes Radio Telescope (right). This relies on accurate laboratory measurements of the molecular lines over a wide range of frequencies. In this project you will measure the rotational spectrum of astronomically important molecules using the UNSW microwave spectrometer and the high resolution FTIR spectrometer at the Australian Synchrotron. You will use these data to produce accurate models for use in finding these molecules in space.



Comparison of observed astronomical spectrum (black) to simulated spectrum based on laboratory data (red) from Lykke et al. A&A 597, A53 (2017).

PROF. JONATHAN MORRIS

Level 2, Dalton Building (F12)

T: 9385 4733 E: jonathan.morris@unsw.edu.au

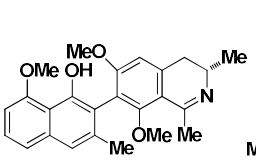
SYNTHETIC AND MEDICINAL CHEMISTRY

- 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.

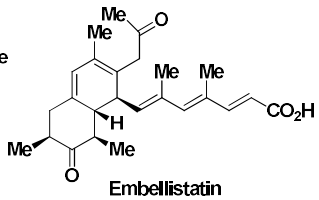
It would be great to work with Honours students on the following projects:

(a) Total Synthesis of Biologically Active Natural Products

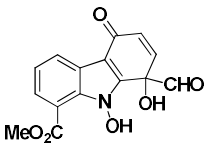
The development of efficient syntheses of biologically active natural products continues to be a major activity of the Morris group, with recent targets including ancistrotanzanine A, embellistatin and coproverdine. As syntheses of these targets are completed, work is initiated on their mode of action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



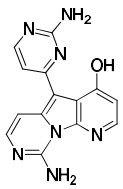
Ancistrotanzanine A



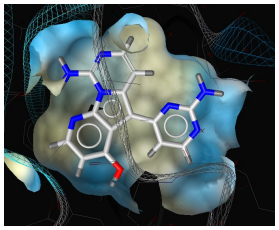
Embellistatin

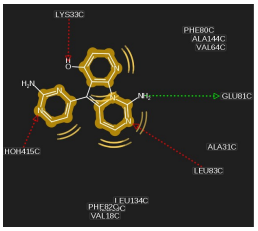


Coproverdine



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

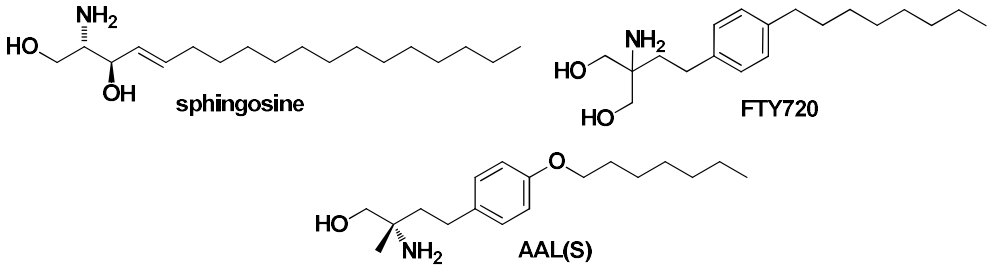
mediate the phosphorylation. This work originated from earlier work on the synthesis of a natural product. Variolin B is a member of a unique class of marine alkaloids isolated from an extremely rare Antarctic sponge. It is no longer available from its natural source. The Morris group have devised a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

A/PROF. SUZANNE M. NEVILLE

Level 2, Dalton Building (F12)

T: 9385 4752 E: s.neville@unsw.edu.au

COORDINATION COMPLEX CHEMISTRY

Our research focuses on exploiting the flexibility of coordination chemistry to explore and develop *molecular switching properties* in polymeric metal-organic complexes. We focus on a type of molecular switching process called 'spin crossover' where two distinct electronic states can be accessed by temperature or pressure variation and light-irradiation. This fascinating process is accompanied by distinct changes in structure, colour and magnetic signal with potential application in data storage, display and sensing industries.

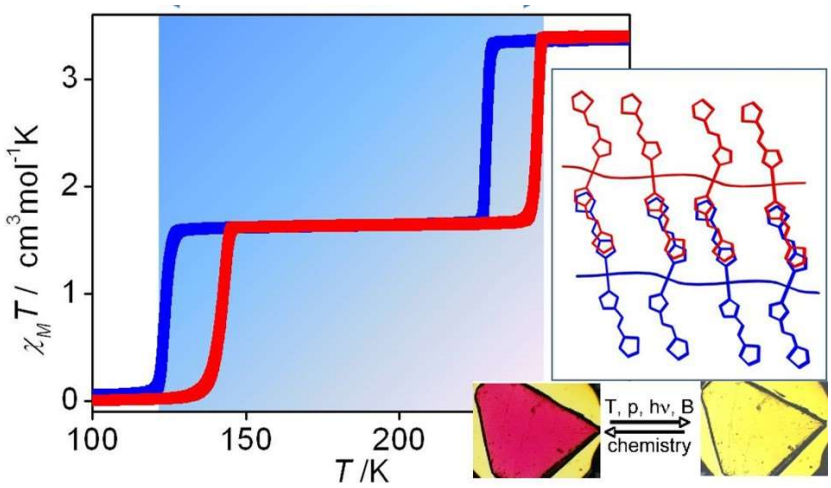
Skills you will learn:

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

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

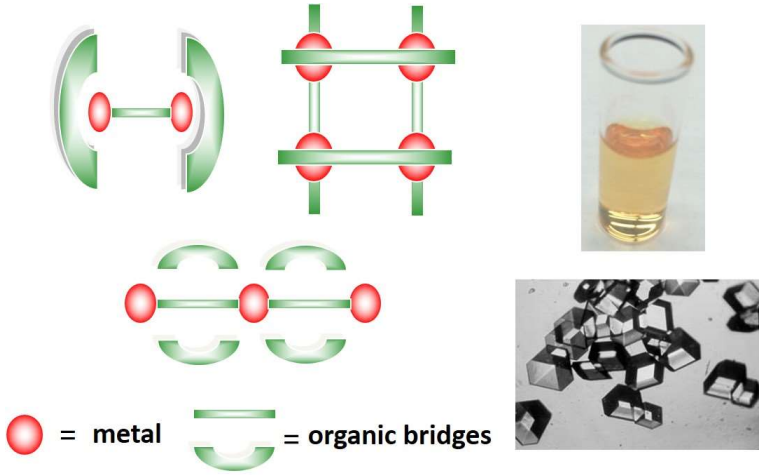
(a) Functional coordination polymers

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



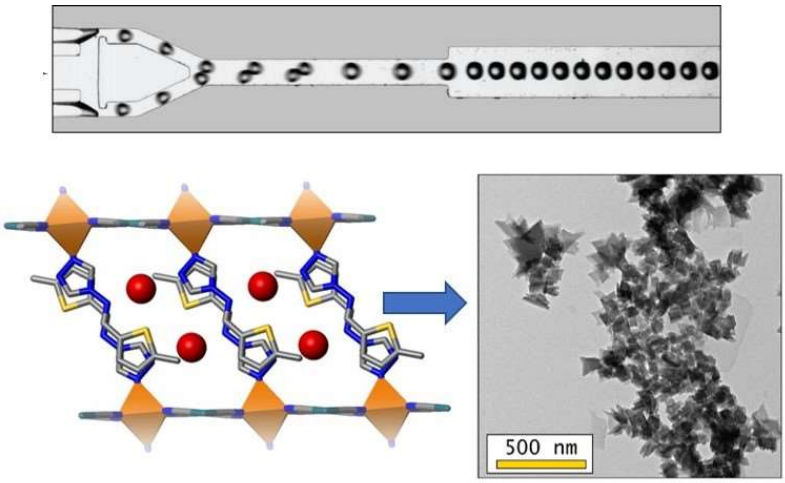
(b) Switchable square and cage complexes

Molecular squares and cages are constructed by the molecular building block approach ("molecular lego"!). In this project we use pre-designed building blocks (metals and ligands) to form, for example, dinuclear, square and cage complexes. The focus will be on including d^{4-7} transition metal ions which can be converted between high and low spin states by temperature, pressure and light-irradiation and investigate switching properties in both solution and solid state (*aka* beautiful crystals!).



(c) Molecular switching nanocrystals

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



DR. VINH NGUYEN

Level 2, Dalton Building (F12)

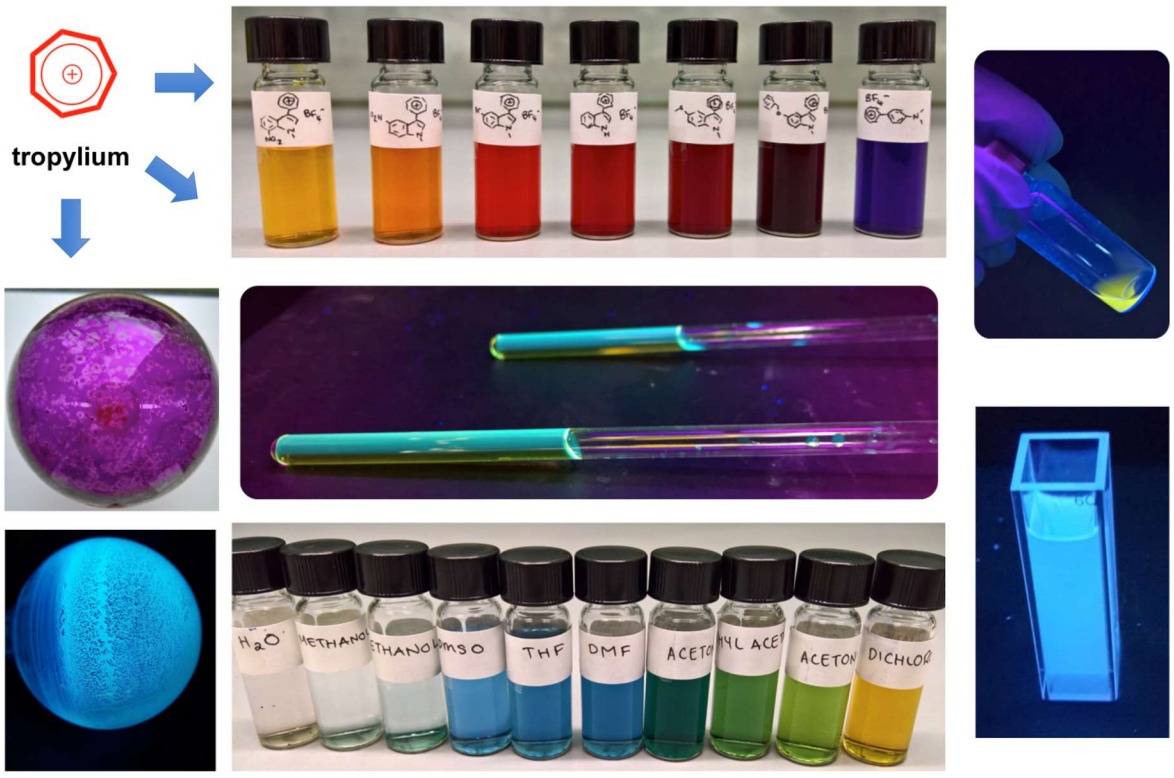
T: 9385 6167 E: t.v.nguyen@unsw.edu.au

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

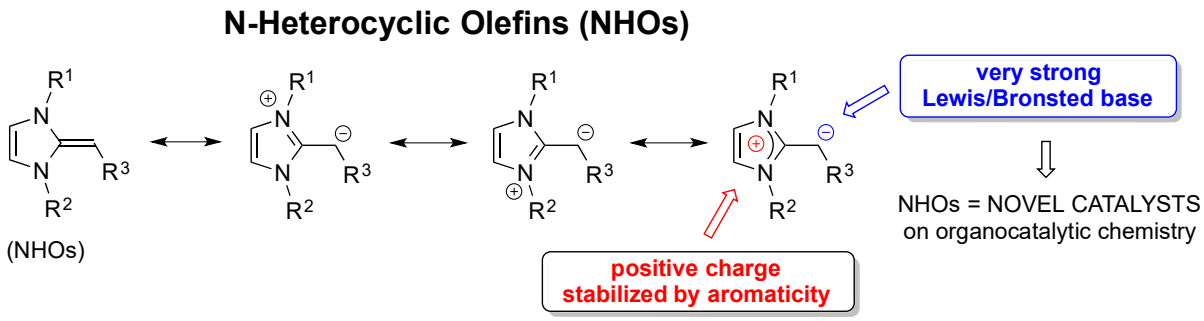
Tropylium ion is an unusual non-benzenoid aromatic system with 6π-electron 7-carbon-ring structure.[1] Recent synthetic advances by our group have made this unique species much more accessible and understood, allowing us now to start to utilize it for a wide range of applications in organocatalytic chemistry[2-5]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

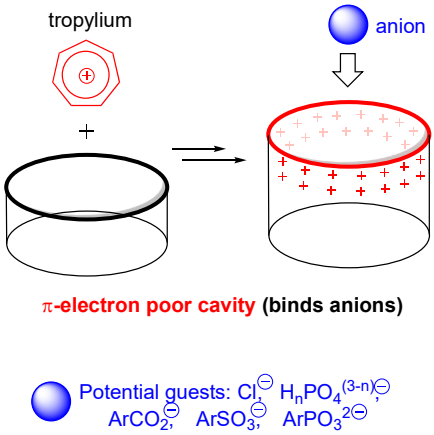
Recently, N-Heterocyclic Olefins (NHOs, see scheme) have emerged as a new class of valuable reaction promoters with interesting action mechanisms. These compounds can be conveniently produced from commercially available precursors in one step. NHOs were originally targeted as a series of active agrochemicals 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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[1] D. J. M. Lyons, R. D. Crocker, M. Blümel, **T. V. Nguyen**,* *Angew. Chem. Int. Ed.* **2017**, *56*, 1466-1484. http://dx.doi.org/10.1002/anie.201605979

[2] **T. V. Nguyen**,* A. Bekensir, *Org. Lett.* **2014**, *16*, 1720-1723. http://dx.doi.org/10.1021/ol5003972

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

[4] **T. V. Nguyen**,* D. J. M. Lyons, *Chem. Commun.* **2015**, *51*, 3131-3134. http://dx.doi.org/10.1039/C4CC09539A

[5] Demelza J. M. Lyons, Reece D. Crocker, Dieter Enders, **Thanh V. Nguyen**,* *Green Chem.* **2017**, in press (DOI = 10.1039/C7GC01519D). http://dx.doi.org/10.1039/C7GC01519D

[6] R. D. Crocker, **T. V. Nguyen**,* *Chem. Eur. J.* **2016**, *22*, 2208-2213. http://dx.doi.org/10.1002/chem.201503575

[7] M. Blümel, J.-M. Noy, D. Enders, M. H. Stenzel, **T. V. Nguyen**,* *Org. Lett.* **2016**, *18*, 2208-2211. http://dx.doi.org/10.1021/acs.orglett.6b00835

[8] M. Blümel, R. D. Crocker, J. B. Harper, D.Enders, **T. V. Nguyen**,* *Chem. Commun.* **2016**, *52*, 7958-7961. http://dx.doi.org/10.1039/c6cc03771b

[9] Ugur Kaya, Uyen P. N. Tran, Dieter Enders, Junming Ho, **Thanh V. Nguyen**,* *Org. Lett.* **2017,** *19*, 1398–1401. http://dx.doi.org/10.1021/acs.orglett.7b00306

CONJOINT A/PROF. GIANCARLO PASCALI

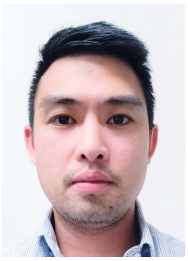
E: g.pascali@unsw.edu.au

Radiochemical innovations

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

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

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



CONJOINT LECTURER, DR JOHN DOAN

T: 9382 2200 E: john.doan1@unsw.edu.au

Radiopharmaceutical Development

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

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

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

DR. MARTIN D. PEEKS

Room 219, Level 2, Dalton Building (F12)

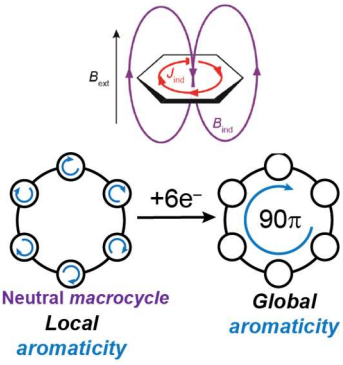
E: m.peeks@unsw.edu.au

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:

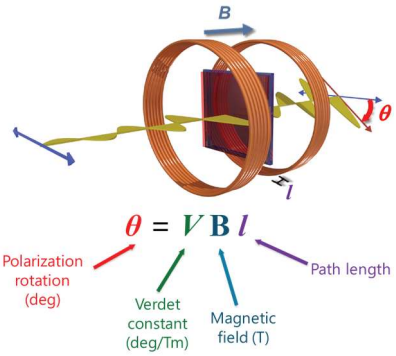
(a) Pushing the limits of π-conjugation, aromaticity, and antiaromaticity



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.

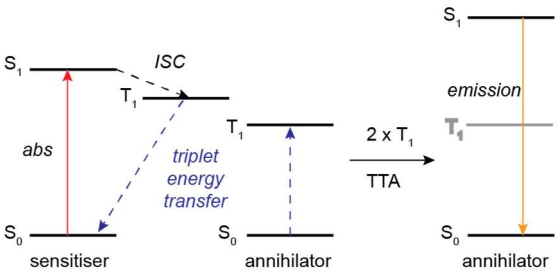
Despite the Faraday effect's ubiquity, it's actually quite weak in most materials, except some ferrimagnetic garnet materials – or that was the prevailing wisdom. Recently it's been discovered that a range of organic materials, from polymers through to liquid crystals, exhibit extreme Faraday rotation.[2]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

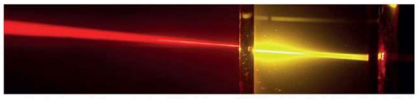
from this initial discovery is to learn *how molecular structure controls* the Faraday rotation. With that knowledge, we will be able to logically design new materials with possible applications in healthcare, self-driving vehicles, and photonics/spintronics.

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.

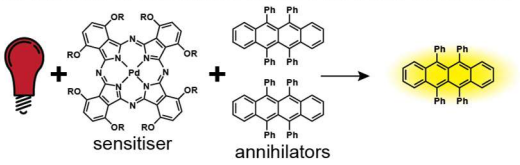
(c) Molecules and assemblies for photon upconversion (with Prof. T. Schmidt)

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

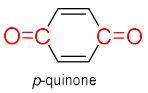


Photon upconversion requires the complex interplay of several different chromophores and their excited states. The relative arrangement of these chromophores in space, as well as their identities, is key for successful upconversion.[4]

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.

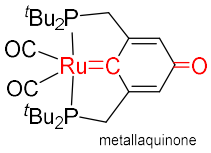
(d) Metal-to-metal communication through cross-conjugated frameworks (with Prof Les Field)

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.

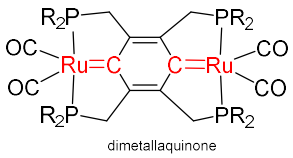


p-quinone

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.

DR. NICOLE J. RIJS

Level 7, Hilmer Building (E10)

T: 9385 7876 E: n.rijs@unsw.edu.au

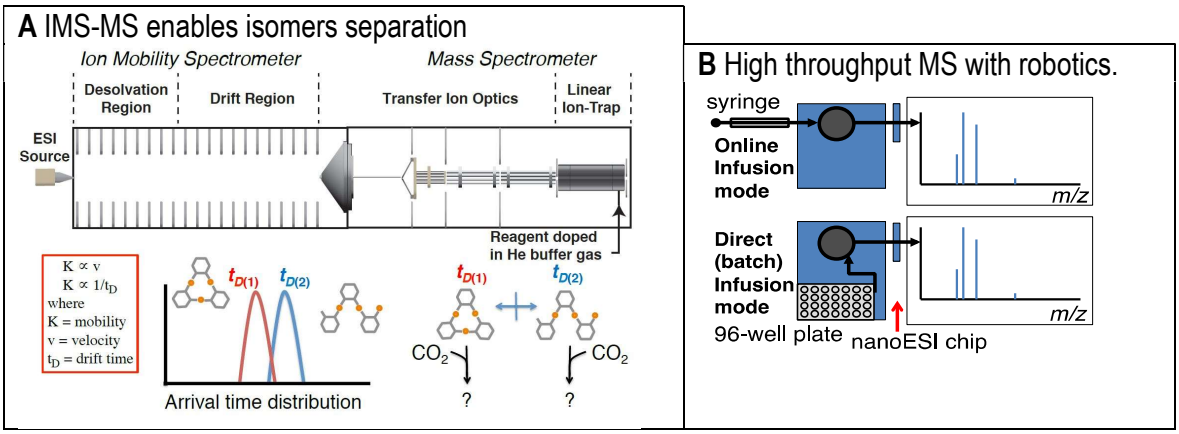
STRUCTURAL CHEMISTRY WITH MASS SPECTROMETRY & ION-MOBILITY

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

Electrospray ionization-mass spectrometry (ESI-MS) is an effective technique for characterising reaction intermediates in synthetic and catalytic transformations. Additionally, ion-mobility spectrometry (IMS) has emerged as a very powerful technique for examining structure. IMS is ideal for examining the size and shape of non-covalent complexes. It offers the advantage of isomer separation on the millisecond timescale, and measurement of the assembly's topology, and as such, enables the study of conformational dynamics within that time frame e.g. monitoring the progress of molecular self-assembly reactions. Together ESI-MS and IMS represent two complementary analytical methods of monitoring reaction solutions on a millisecond timescale.

Unique techniques used in the Rijs group include:

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



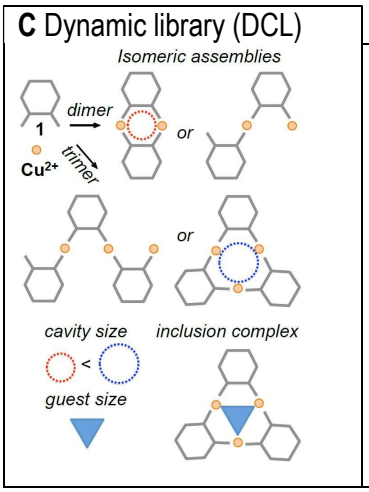
It would be great to work with students on the following projects:

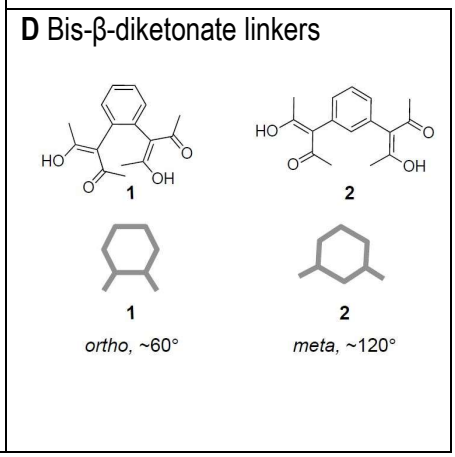
(a) Intercepting critical intermediates from dynamic combinatorial libraries of bis-β-diketonates

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

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

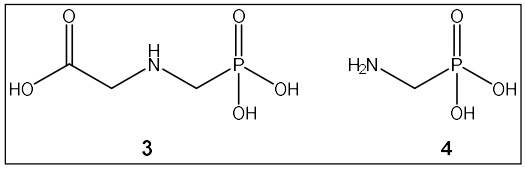
The aim of this project is to develop a methodology for monitoring self-assembly and to direct the synthesis of selective uptake assemblies. Robotically controlled nESI-MS will be used to measure the stoichiometry of evolving molecular assemblies, formed from DCLs.





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

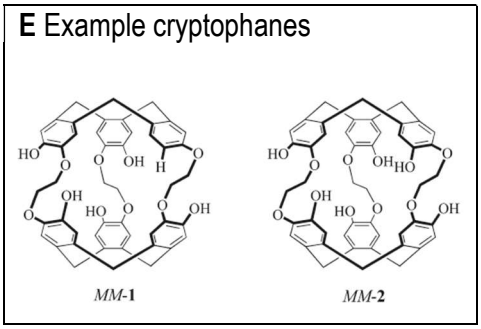
N-(phosphonomethyl)glycine, commonly known as Glyphosate, is a ubiquitous herbicide worldwide. Aminomethylphosphonic acid (AMPA) is the main metabolic product of glyphosate. Metal complexation of this herbicide and its degradation product is an important factor affecting the environmental fate in soil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



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

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

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



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

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

DR. FELIX RIZZUTO

Arriving in 2022

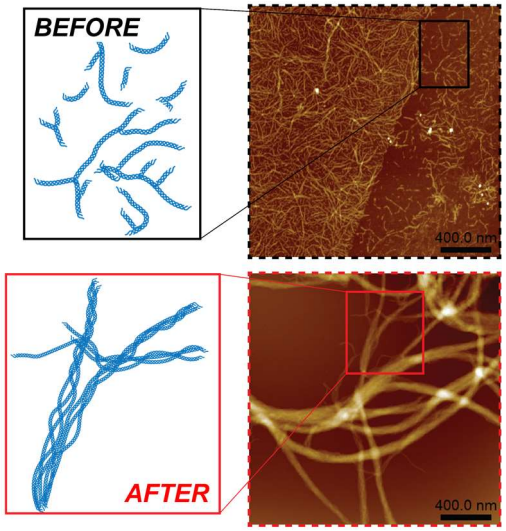
E: felix.rizzuto@gmail.com

SOFT NANOMATERIALS AND SYSTEMS CHEMISTRY

Our research looks at new ways of synthesising and manipulating soft materials. 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, nanomaterials evolution. We are a new group joining UNSW in 2022: feel free to email or DM me on twitter if you have any questions!

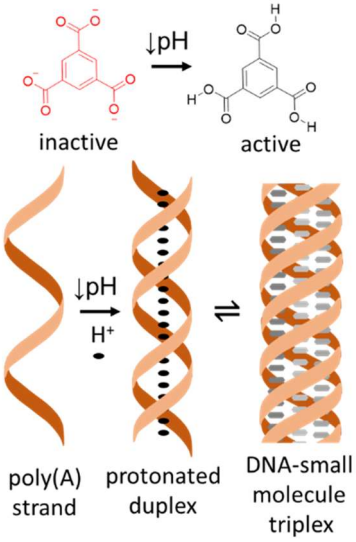
It would be great to work with Honours students on the following projects:

(a) Making 'perfect' nanomaterials



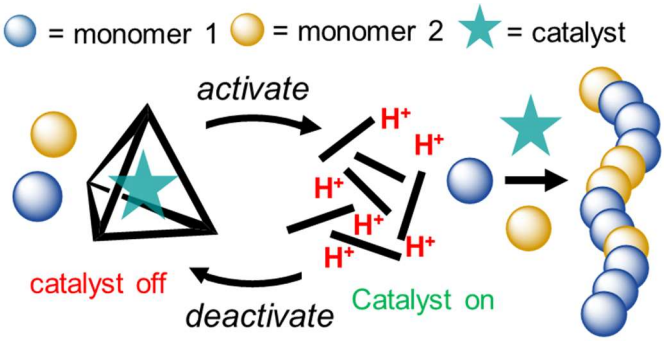
No material is perfect – even the most robust can have defects, cracks and scars at the nanoscale. We can tune the energy landscape of materials assembly by 'pushing' these structures away from their equilibrium positions. As these systems relax to their energy minima, components are released slowly, healing defects and producing more structured and higher-performance nanomaterials. In this project we will develop new pathways for using chemical fuels and light-activated switches that rip nanomaterials apart. We will regulate self-assembly pathways and direct the formation of new and functional nanomaterials. A sample of what we can currently do is shown to the right – using this technology we can modulate the properties of polymers, converting highly interwoven materials (before) into nanocable superstructures (right).

(b) Self-assembled polymers based on 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 new structures to build 2 and 3 dimensional constructs that we can image using state-of-the-art microscopy techniques.

(c) 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.

Skills learnt in my group: Non-covalent chemistry, polymer chemistry, self-assembly, metal-organic assembly, stimuli-responsive nanomaterials, microscopy, biomaterials analysis.

Relevant publications: ***Nat. Chem.***, 2021, DOI: 10.1038/s41557-021-00751-w, in press; ***Nat. Mater.***, 2020, 19, 1012-1018; ***Chem. Soc. Rev.***, 2020, 49, 4220-4233; ***Nat. Rev. Chem.***, 2019, 3, 204-222.

PROF. TIMOTHY SCHMIDT

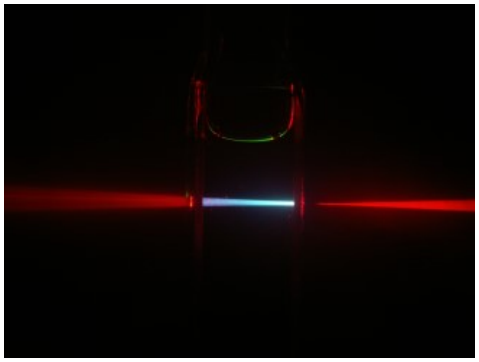
Level 5, Science and Engineering Building (E8)

T: 04 39 386 109 E: schmidtim@gmail.com

MOLECULAR SPECTROSCOPY AND SOLAR ENERGY

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

(a) Photochemical Upconversion for Improved Solar Energy Conversion



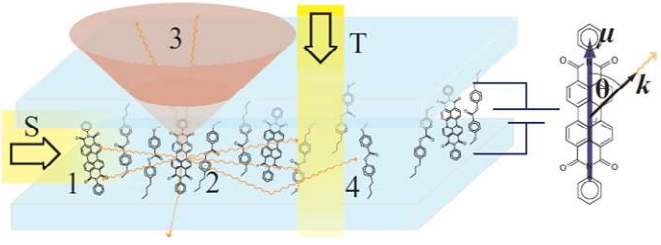
Light from the sun reaches us as a continuous spectrum. But, to generate a photovoltage in a solar cell, we usually neglect that part of the spectrum with photon energies below the band gap. Such a strategy limits the energy conversion efficiency of solar cells to about 33% (UNSW Si cells have reached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

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

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

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

When light falls on a slab of material containing fluorophores, light is absorbed but re-emitted *isotropically*. About 75% of this light is trapped in the slab by total internal reflection, and guided towards solar cells on the edge of the slab. Until now, such systems have been plagued by reabsorption effects. We will couple fluorescent dyes to light-absorbing nanomaterials to separate the roles of absorption and emission, and reduce reabsorption. Further improvements have been shown by us to be possible by clever design of the orientation of transition dipole moments.

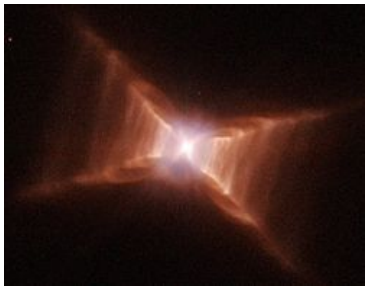


(c) Laser Spectroscopy of Isolated Radicals and Ions (with Prof. Scott Kable)

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

Atmospheric Radicals

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



Interstellar Molecules and Ions

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

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

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

(d) Advanced Spectroscopy for Complex Functional Materials (with Dr Dane McCamey, School of Physics)

Complex functional materials are employed in a range of applications, the development of which is motivated by the future technological needs of society. Organic solar cells, organic light emitting diodes and organic electronics all employ materials characterized by a complex relationship between morphology and function which can only be elucidated by advanced spectroscopic techniques.

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

A/PROF. NEERAJ SHARMA

Dalton Building (F12)

T: 9385 4714 E: neeraj.sharma@unsw.edu.au

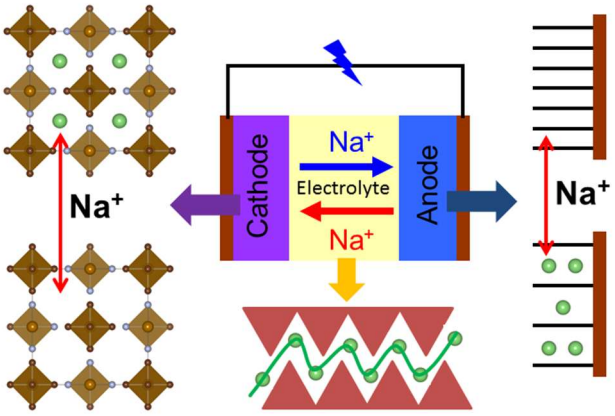
SOLID STATE AND MATERIALS CHEMISTRY

- 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

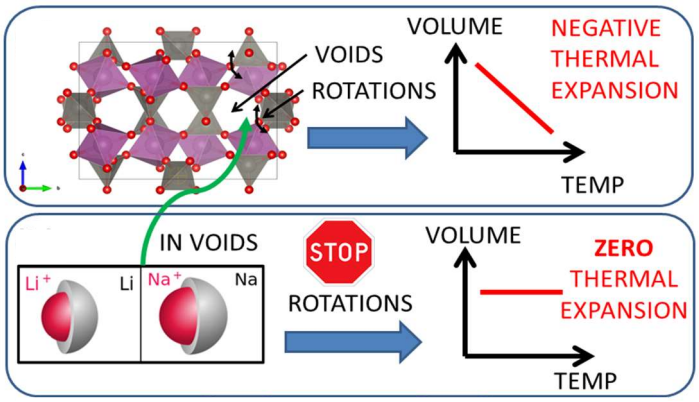
Sodium-ion conducting ceramics or glassy-ceramics are known to be excellent electrolytes at high temperatures (>300°C). This project works towards making materials with sufficient sodium-ion conduction at room temperature.

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.

SCIENTIA PROF. MARTINA STENZEL

Level 7, Science and Engineering Building (E8)

T: 9385 4656 E: m.stenzel@unsw.edu.au

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:

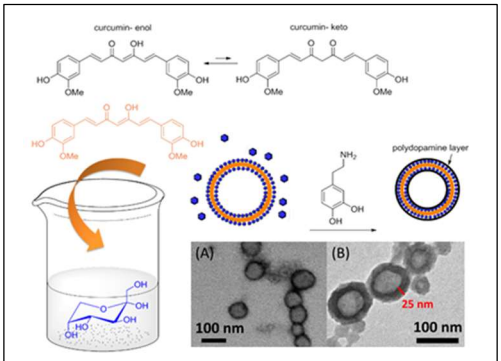
(a) Making polymers

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.

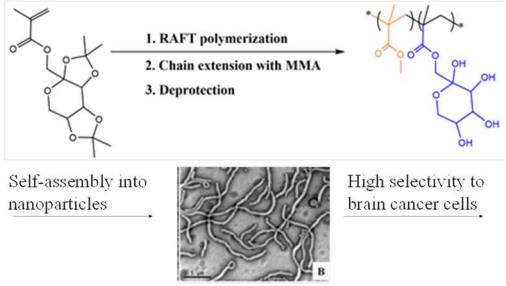


Nanocapsule by mixing of curcumin and sugars, stabilized by a polydopamine shell

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.

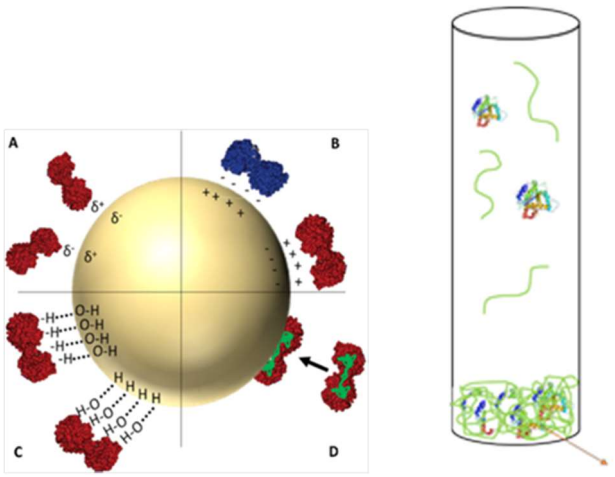


Synthesis of glycopolymers and their self-assembly into nanoparticles

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.

A/PROF. JOHN STRIDE

Level 1, Dalton Building (F12)

T: 9385 4672 E: j.stride@unsw.edu.au

MATERIALS CHEMISTRY AT THE NANOSCALE

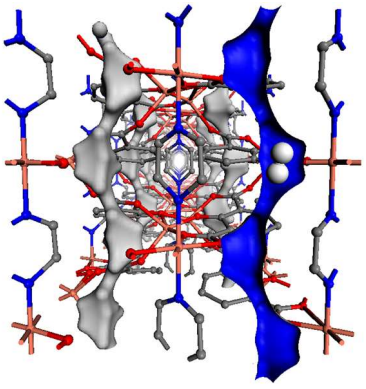
My group focuses on making and understanding new materials that are often focused on some of the major challenges facing us today: energy, water and sustainability. We make use of a range of techniques that include X-ray and neutron scattering in truly multi-disciplinary projects. Key to these studies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

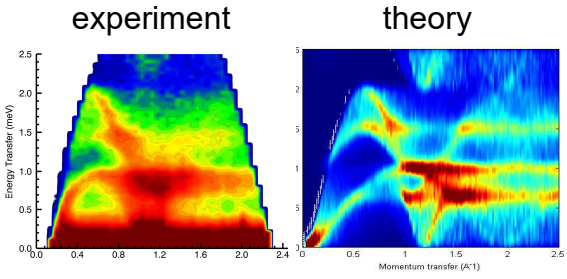
Sorting and storing molecules - how to select for one molecule over another



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

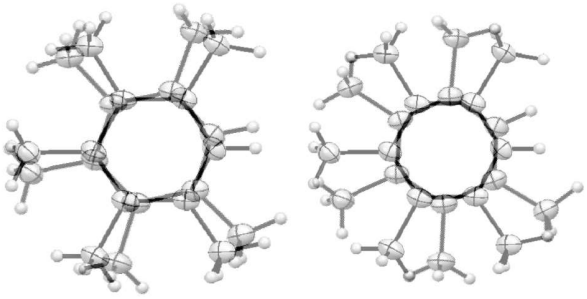
Magnetic materials have revolutionised the way in which we store and use information and have a key role to play in quantum computing; they have also been a navigational aid for centuries and are even pretty useful at securing notes to the fridge door. It is fascinating therefore that we still do not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



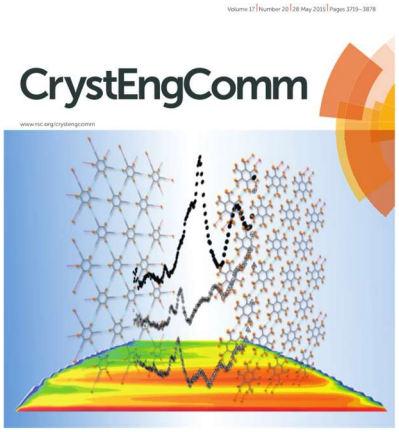
(a) crystalline phase (b) plas1c phase

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.

DR. SCOTT A. SULWAY

Level 1, Dalton Building (F12)

T: 9385 5236 E: s.sulway@unsw.edu.au

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.

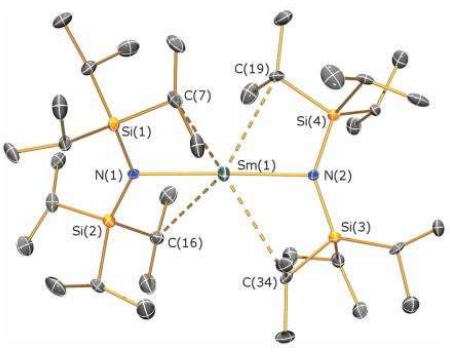
Skills you will learn:

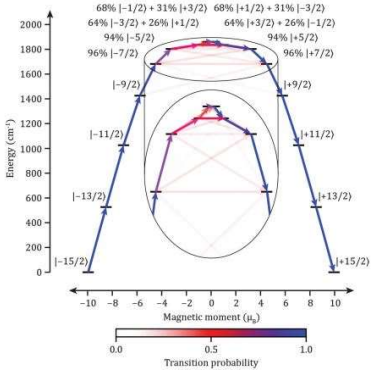
- Manipulation of air- and moisture-sensitive compounds
- Organic and Inorganic synthetic chemistry
- Structure elucidation – NMR spectroscopy (^{1}H, ^{13}C), IR spectroscopy, SQUID magnetometry and XRD (Yeap, we grow crystals)!

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

(a) Sterically hindered low-coordinate lanthanide compounds

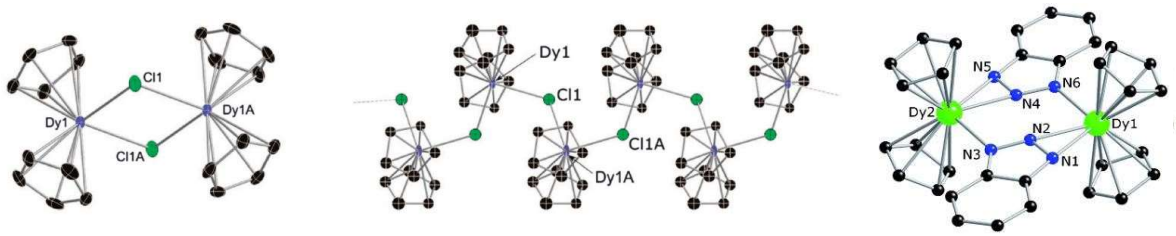
Recent insight into stabilisation of the m_J states of lanthanide containing compounds hints at the potential ability to synthesis compounds that have higher energy barriers to magnetic relaxation than any 3d-block compound. It has been suggested that even subtle changes to the coordination environment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

PROF. PALL (PALLI) THORDARSON

Level 7 (Room 741), Hilmer Building (E10)

T: 9385 4478 E: p.thordarson@unsw.edu.au

RNA CHEMISTRY, ORIGIN OF LIFE AND NANOMEDICINE

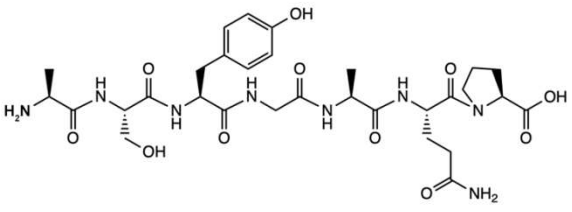
- **RNA Chemistry** with focus on understanding how RNA interacts with peptides other molecules and how these interactions can be applied in RNA science and therapeutics
- **Origin of Life and Systems Chemistry,** exploring the role of self-assembly in how life originated and how we can make life-like 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).*

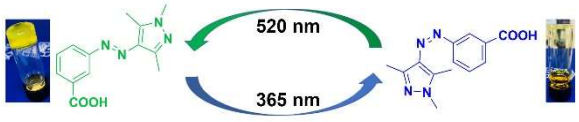
Peptides/proteins and RNA are two of the key building blocks of life. Recently it has become proteins and RNA drive the formation of lava lamp or vinaigrette "droplets"[1] within the cell but biologists are now just uncovering now how important droplet- or gel-like protein-RNA complex are in biology 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 Dr T. Vinh Nguyen, A/Prof. Jonathon Beves and A/Prof. Kris Kilian, School of Chemistry).*

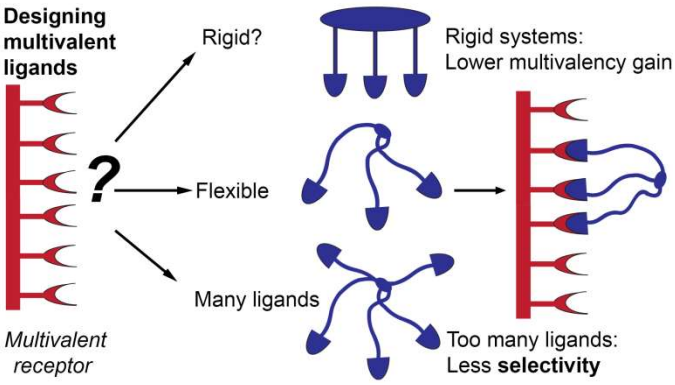
Self-assembled peptide gels have already been proven to be useful as 3D material for growing living cells, even neurons.[4] We have extended this work to include the formation of gels that can changed through a photo-switch,[5] or mixing with a biological material such as collagen. In more recent work 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) Multivalency in drug delivery and protein-protein interactions *(collaboration with A/Prof. Joshua McCarrol and Prof. Maria Kavallaris, Children's Cancer Institute Australia).*

How does the Gecko walk up a wall? How do you stop an influenza virus from binding to and infecting their target cells? The answer to these very different questions centres on the same topic – multivalency! Essentially you need to get a lot of weak interactions to work together, to creating a large effect. The multivalency is also strongly related to another very important topic in biology and supramolecular chemistry - cooperativity.[6]

Despite being known for decades, we still fully understand how the multivalency effect really works on the molecular level and how it can be used to more effectively treat diseases, be it influenza or cancer.[5] But even making a "dimeric" or a "tetrameric" copy of a targeting ligand such as a peptide can have pronounced biological effect – sometimes as much as changing the activity by a 10-1000 fold! Building on recent theoretical advances, we have now a framework (see Figure)[7] to design more effective multivalent system. Projects involving cancer cell targeting[8] and better control over protein-protein interactions, which are important in many diseases ranging from Alzheimer to cancer, are available for anyone that wants to combine synthetic chemistry, supramolecular chemistry and medicinal chemistry in their research training.



1. Elie Dolgin. Cell biology's new phase. *Nature*, **2018**, *555*, 300-302.
2. Pall Thordarson. "Emergence of Life" in *Encyclopedia of Supramolecular Chemistry*: eds: Jerry L. Atwood, Jonathan W. Steed, Marcel Dekker Inc., New York, **2004**, 528-534.
3. Martin Van Kranendonk, David W. Deamer and Tara Djokic, Life Springs, *Scientific American*, August **2017**, 28-35.
4. 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. Larissa K. S. von Krbek, Christoph A. Schalley and Pall Thordarson. Assessing cooperativity in supramolecular systems, *Chemical Society Reviews*, **2017**, *46*, 2622-2637.
7. Kristel C. Tjandra and Pall Thordarson, Multivalency in Drug Delivery – When Is it Too Much of a Good Thing? *Bioconjugate Chemistry*, **2019**, *30*, 503-514.
8. Kristel C. Tjandra, Nigel McCarthy, Lu Yang, Alistair J. Laos, George Sharbeen, Phoebe A. Phillips, Helen Forgham, Sharon M. Sagnella, Renee M. Whan, Maria Kavallaris, Pall Thordarson and Joshua A. McCarroll. Identification of Novel Medulloblastoma Cell-Targeting Peptides for Use in Selective Chemotherapy Drug Delivery. *Journal of Medicinal Chemistry*, **2020**, *63*, 2181-2193.

PROF. RICHARD TILLEY

B89, Chemical Sciences Building (F10)

T: 9385 4435 E: r.tilley@unsw.edu.au

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.

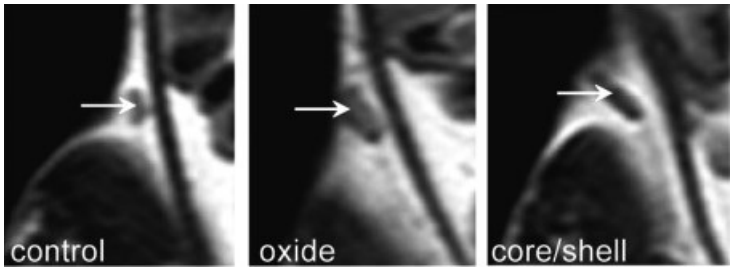


Figure 1: MRI images from iron nanoparticles injected into a mouse to enhance the contrast of a tumour.

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.

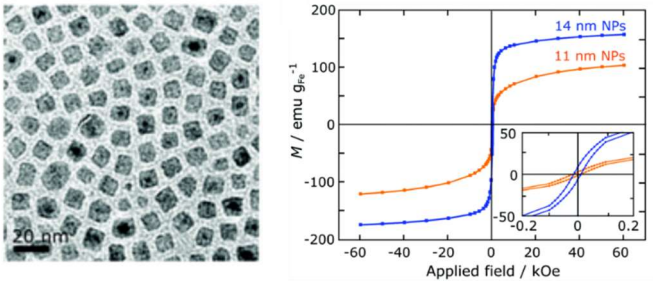


Figure 2: Transmission electron microscopy images of iron nanocubes and their magnetic properties for use in MPI.[1]

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).

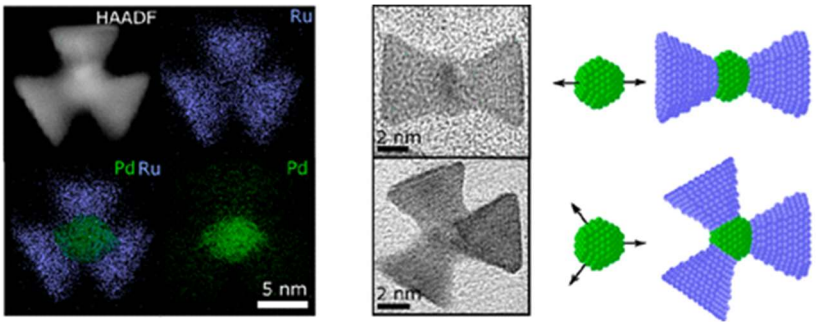


Figure 1: Energy dispersive X-ray spectroscopy elemental mapping of Pd-Ru branched nanoparticles and TEM images of individual nanoparticles. Models show the controlled direction of growth of Ru from Pd seed.

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]

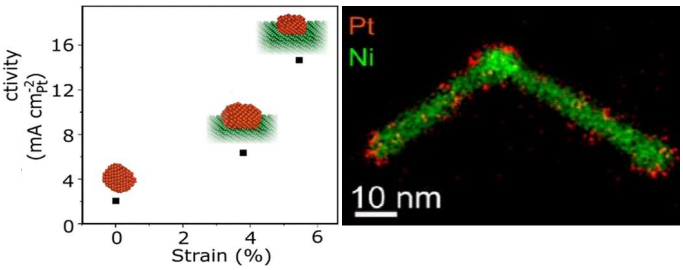


Figure 1: Relationship between strain and HER activity and elemental map of a Pt on Ni nanoparticle.[2]

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

Office: Level 7, Hilmer (E10) | Lab: Level 6, SEB (E8)

E: anna.wang@unsw.edu.au | annawanglab.com

SOFT MATTER BIOPHYSICS AND THE ORIGINS OF LIFE

- We tackle problems at the nexus of chemistry, physics, biology, and materials science.
- Students with chemistry, medicinal chemistry, and other backgrounds are all welcome – 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 Google.

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

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

The mechanical environment of cells often determine 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.

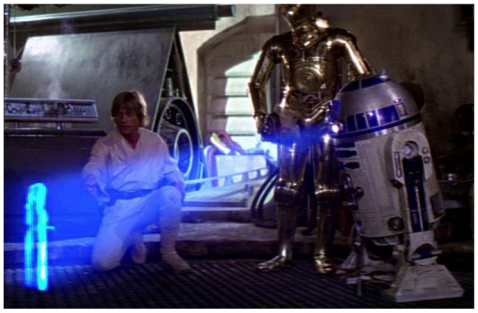


Fig. 1 "Holographic imaging" in the movies

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

(b) Membrane fusion for origins of life and drug delivery

A lipid bilayer encases each of our cells. Lipids are also used for drug delivery e.g. mRNA vaccines. How can we control the fusion of lipid compartments by modulating their composition? The answers to this question are important for targeted drug delivery, and would also help us understand how evolution could have been kickstarted at the origins of life.

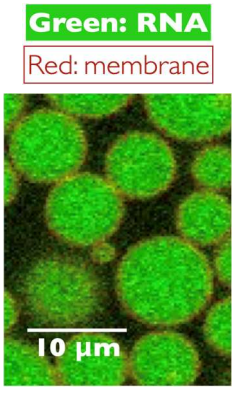


Fig. 2 Liposomes containing RNA

Fusion rates will be monitored by mixing two populations of vesicles labelled with different dyes, and using epifluorescence microscopy to monitor fusion over time. Students will also use electrical impedance spectroscopy and fluorescent probes to monitor lipid particle properties as a function of composition.

(c) Fluidity of a growing synthetic cell

This project is part of an international collaboration with labs in the US and Japan.

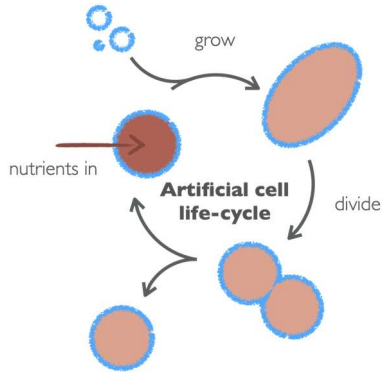


Fig. 3 A dynamic growing system

Cells typically have a fluid phospholipid membrane that grows and divides in order for a cell to propagate. Can we recreate this process in a synthetic cell?

This project will investigate how the intermediates of lipid synthesis, including lysophosphatidic acids and fatty acids, affect the fluidity of membranes. Do the precursors make the membrane more or less fluid? How is the lipid packing altered? These results will be applied to designing a synthetic biology system that can continually grow and divide, to make more of itself without intervention.

(d) Characterising liquid-liquid phase separation with holographic microscopy (in collaboration with Prof. Pall Thordarson)

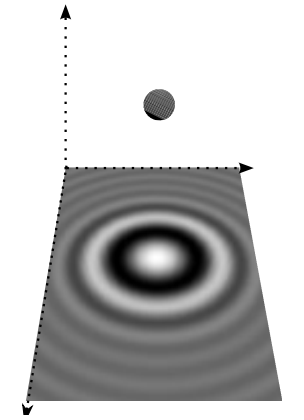


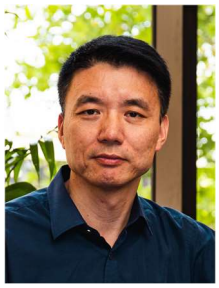
Fig. 4 Hologram of droplet

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.

It is critical to a variety of fields to understand and 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.

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

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



PROF. CHUAN ZHAO

Level 1, Room 127, Dalton Building (F12)

T: 9385 4645 E: chuan.zhao@unsw.edu.au

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.

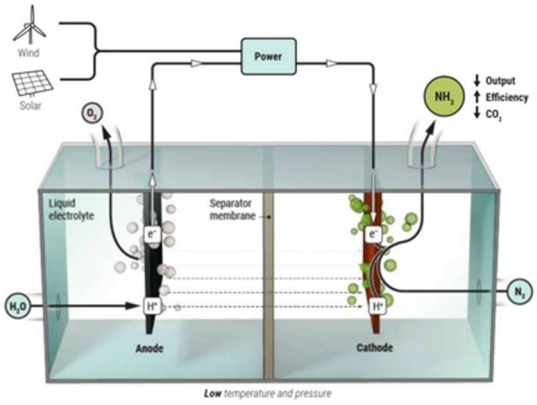
It would be great to work with Honours students on the following projects:

(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**

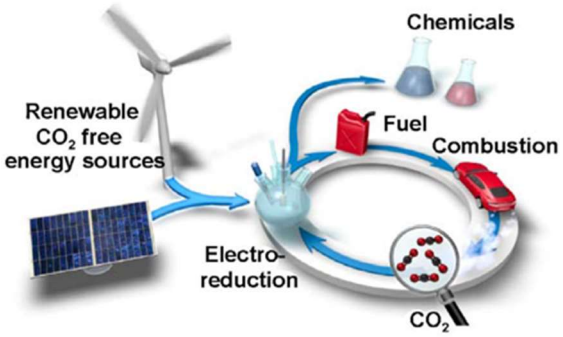
Ammonia (NH_3) is one of the most important and widely produced chemicals worldwide for fertiliser production and is also a promising liquid hydrogen carrier to be used as a carbon-free fuel. N_2 has a very strong triple bond and is extremely inert. Currently, the synthesis of NH3 is still dominated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