

2021 Discipline of Chemistry (MLS)

Honours Research Projects Booklet

October 16th 2020

TABLE OF CONTENTS

Welcome, Honours Course Work, Honours Timeline	<i>i</i>
Honours coordinator details	<i>iii</i>
Selection of Honours Research Projects	<i>iv</i>
List of Honours Research Projects	1 – 21
 Projects Classified by Sub-Discipline	
Analytical Chemistry	1, 2, 6, 8, 10, 13, 20, 22
Inorganic Chemistry	9, 16, 17
Organic Chemistry	7, 14, 18,
Physical Chemistry	3, 4, 5, 9, 11, 12, 15, 16, 19, 20
Chemistry Education	21
 Projects Classified by Area of Application	
Biological/Medicinal	7, 8, 15, 16, 18
Computational	4, 5, 12, 15, 19
Education	21
Environmental	6, 8, 22
Forensic	13, 20
Nano/Sensors/Surfaces	2, 3, 9, 11, 20
Synthesis	7, 9, 14, 16, 17, 18
Water Chemistry	1, 2, 10

Welcome To Chemistry Honours

1.1 Chemistry Honours Enrolment

By University Rules, students must have completed a BSc and have a year weighted average in third year of 65% or more to be eligible for Honours. Hence you do need to graduate!! All eligible Honours students will be admitted to the one year BSc Honours course, BH-SCNCE, majoring in chemistry. Follow the process described at: <http://graduations.curtin.edu.au/graduate/how.cfm>.

Note: This is not the case for Advanced Science Students, for which the Honours is embedded in the 4-year Advanced Science degree.

All students will enrol in Chemistry Honours Dissertation (CHEM4000, Full Year, 150 credits), Advanced Topics in Chemical Analysis and Spectroscopy (CHEM4002, Trimester 1, 25 credits), and Advanced Topics in Chemistry (CHEM4001, Trimester 1, 25 credits). If you would like to be considered for Chemistry Honours admission please apply here: [http://courses.curtin.edu.au/course overview/undergraduate/science-honours](http://courses.curtin.edu.au/course%20overview/undergraduate/science-honours). The Student Services Office will contact the Honours Coordinator for approval of eligibility once the exam results have been confirmed, and then the enrolment process will be initiated. Feel free to contact the Honours Coordinator, or the Student Services Office, if you are concerned about your enrolment.

1.2 Advanced Topics in Chemistry - CHEM4001

Advanced topics in chemistry will be studied to illustrate how fundamental aspects of chemistry underpin the cutting edge of knowledge and research in a wide range of scientific disciplines and applications. Methods that can be used to communicate advanced chemical concepts will be discussed and implemented.

Tuition pattern (weekly): 2 hours lecture + 2 hours workshop.

Assessment: Mid-semester exam, Final exam, oral exam.

1.3 Advanced Topics in Chemical Analysis and Spectroscopy - Chem4002

This unit will impart skills in independent manipulation of techniques in chemical synthesis, analysis, and computation. Students will solve a problem, first using practical techniques of relevance to the task, and then interpreting the outcome using computational techniques. To achieve these goals, students will be inducted into research laboratory practices by applying electronic note keeping and appropriate occupational health and safety procedures.

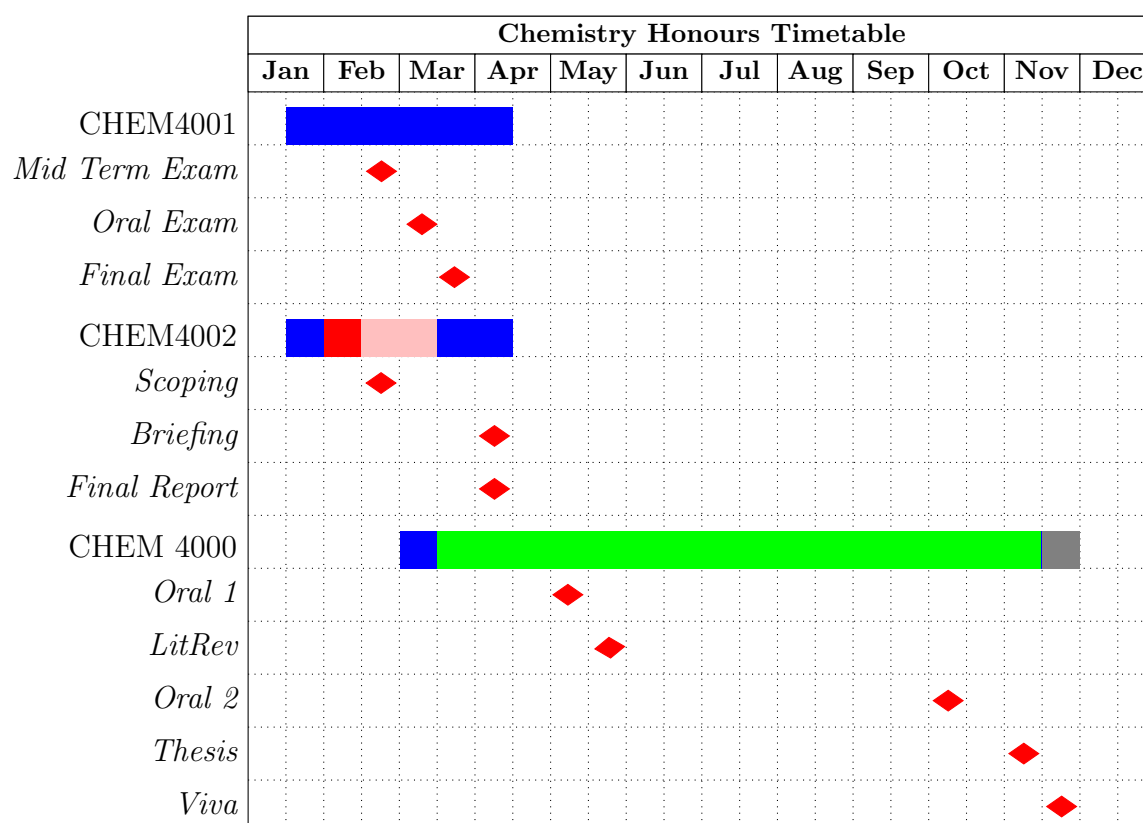
Tuition pattern: 1 hour seminar weekly, 5x6 hours chemistry lab (over 2 weeks) , 4x2 hours computer lab (over 4 weeks).

Assessment: assignment, oral exam, final report/lab book.

1.4 Chemistry Honours Dissertation - CHEM4000

Students will be required to conduct an independent research project in the chemical sciences under the guidance of a supervisor, resulting in the preparation, submission, presentation and defence of a dissertation. Students will develop research, technical and professional and communication skills, research autonomy and specialised knowledge through a process of inquiry involving the formulation of research questions and hypotheses; selection of appropriate methodology and experimental design; ethical consideration of the research process; critical review of scientific literature; effective scientific writing; development of a project proposal, and the preparation of a dissertation. Assessment: two oral presentations, seminars reflections, draft report, final report, viva.

1.5 Approximate Honours Timeline



The lab work for CHEM400 can be undertaken only during the green portion of the bar. The first 2 weeks, which overlap with the CHEM4001 and CHEM4002 units can be used for Literature Review, Risk assessment and other preparatory work, which do not require access to the labs. The last two weeks (grey band) will be devoted to the preparation for the viva voce examination.

Honours Coordinator (Chemistry)

Dr Mark Hackett

Room: 500-4119

Phone: 9266 3102

E-mail:

mark.j.hackett@curtin.edu.au

CHEM4000 Projects

2.1 Chemistry Honours Projects Allocation

Students should review the list of available Honours projects in this Honours Project Booklet and meet with potential supervisors to discuss the projects on offer, in order to choose their project preferences. Contact details for all Curtin supervisors are provided to assist you in this process. All students are requested to provide six project preferences (in order) to the Honours Coordinator by 30th November 2020. **Only one project from a particular supervisor** may appear in your list of project preferences (i.e. your list of project preferences should include projects from 5 different supervisors). Project allocations will be confirmed as soon as possible, after eligibility can be confirmed. Please provide an email address through which you can be contacted. Allocation of projects will take into account a number of factors, including student merit, student preferences and interests, as well as allocation of students across available supervisors and workload of supervisors. Select your project preferences carefully, keep an open mind and consult as widely as possible. Please note that late submissions and/or incomplete submissions will result in the student being allocated to remaining projects after everyone else has been allocated, irrespectively of the listed preferences.

2.2 Choice of Project

The Chemical Research Methods 3006 Project Booklet has given you specific information about the choice of research projects for your Chemical Research Methods 3006 unit and your Honours year. This information is provided again here: Please note that any Honours project undertaken is required to be substantially different to your Chemical Research Methods 3006 project (and any summer work that you might undertake). When the time comes, you must ensure that any potential overlap is discussed with your Honours supervisor. To assist the Honours Panel to assess the Honours project appropriately, if there is overlap or potential overlap, your Chemical Research Methods 3006 report will need to be submitted with your Honours Thesis. This is designed to ensure that there is a level playing field for all Honours candidates. Please note it is YOUR responsibility (through appropriate discussion with potential supervisor/s) to ensure that your Chemical Research Methods 3006 project and your Honours project are sufficiently different, or that any overlap is brought to the attention of the Honours Coordinator so that it can be managed appropriately.

2.3 Honours Projects Available in 2021

This Honours Project Booklet describes the research projects in the Department of Chemistry, listed under the name of the primary Curtin supervisor, which are available to students enrolling for Honours in 2020. If you have any questions about this process, please contact the Honours co-ordinator.

After you have reviewed the available projects and discussed with the potential supervisor what are the requirements and what is expected from you during the project, please **submit your preferences to the honours coordinator by 30th November**. Please ensure that projects from 6 different primary Curtin supervisors are listed. You can provide the information by using this form, or type ALL the information into an email.

In 2021 students may also propose an Honours projects, outside of those listed in the booklet. The proposed project must be first discussed with the supervisor and Honours coordinator, and is subject to feasibility approval by the Honours Course Coordinator.

Student Name:		Student ID:
Contact email:		Contact Phone:
Project title		Project Supervisor
1		
2		
3		
4		
5		
6		

Dr Sebastien Allard

Office: 500-4113

Lab: 500-3206

Phone: 9266 7949

Email: s.allard@curtin.edu.au



Background

The main focus of my research is water chemistry and the development of innovative analytical methods. I have expertise in oxidation processes, particularly with regards to the kinetics and mechanisms of the degradation of micropollutants. I have developed numerous analytical methods mainly with Gas Chromatography Mass Spectrometry (GC-MS).

Chemical analysis of e-cigarette liquids with A/Prof Alex Larcombe^{1,2}, A/Prof Benjamin J. Mullins². 1.Telethon Kids Institute.2.School of Public Health, Curtin University.

Commercial electronic cigarette liquids (e-liquids) consist of a base of propylene glycol and/or glycerine in various ratios. To this excipient mixture, flavours, nicotine and other chemicals such as flavour enhancers, are added. Of key concern is the presence of nicotine in e-liquids. In many jurisdictions (including Australia), it is illegal to sell e-liquids containing nicotine. Despite this, there have been numerous instances of nicotine being detected in commercially available e-liquids labelled as “nicotine-free” in addition to the level of nicotine in e-liquids being considerably different to that listed on the label. These discrepancies are not surprising due to lack of regulation and quality control in the e-liquid manufacturing industry in which poor-quality counterfeit versions of major brands are common. Of further concern is that other (flavouring) ingredients are generally undisclosed and while many may be “food grade” – they have often not been tested for inhalation toxicology. This work aims to develop novel Solid Phase Microextraction (SPME)-based analytical methods allowing measurement of the main chemicals present in e-liquids including nicotine and other potentially harmful compounds. This will include a range of chemical group including aldehydes, ketones, carboxylic acids, polyaromatic compounds and phenolic compounds.

Degradation of Poly- and per-fluoroalkyl substances by powerful advanced reduction processes (with Manaswini Natarajan)

In this project, we will investigate and optimise destruction technologies that are ex situ including powerful advanced reduction processes (UV/sulphite and UV/Iodide). Advanced reduction processes (ARP) involve the generation of highly reactive and non selective radical like hydrated electrons which can degrade the PFASs. Due to high electronegativity, the fluorine atoms in the PFASs are more amenable to reductive attack rather than oxidative attack. Reductants used for ARPs of PFASs include zero valent iron, UV radiated aqueous iodides, sodium dithionites and sulphites. A typical photoreductive procedure requires a photoreactor and purging with nitrogen or argon gas to remove oxygen. The generation of hydrated electrons (eaq⁻) has been observed in the reductive defluorination of PFAAs, which act on the alpha C-F bond instead of the C-C bond to initiate the defluorination reaction releasing fluoride (Ross, McDonough et al. 2018). In this study a large range of state-of-the-art analytical capabilities will be required. The reactor vessel will consist of a 15 W low-pressure mercury lamp emitting monochromatic UV light at 254 nm. PFAS will be analyzed using LC-MS/MS. UV spectroscopy, HPLC-UV will also be required to complete this work.

Prof. Damien Arrigan

Office: 500-3115

Lab: 500-2222

Phone: 9266 9735

Email: d.arrigan@curtin.edu.au



Background

Our research is focused on analytical chemistry strategies that employ electrochemical reactions, either at liquid-liquid interfaces or at solid electrodes. These methods open up new ways to solve chemical measurement problems in industrial, environmental or biomedical areas. These projects will provide valuable experience in modern electroanalytical chemistry and sensor technology and are tailored to the interests of each student.

Exploring new sensors for PFAS

Per- and poly-fluoroalkyl substances (PFAS) have emerged in recent years as environmental contaminants of great concern due to their persistence and accumulation in the environment. Contamination of soils and groundwaters from use of PFAS materials in fire-fighting foams has resulted in efforts to clean-up such sites. However, lab-based analyses remain the key measurements of contamination and clean-up effectiveness. By using electrochemistry at liquid-liquid interfaces, we have recently been able to detect perfluorooctanesulfonic acid (PFOS) at concentrations lower than 100 picomolar,¹ which indicates that electrochemistry might be a suitable basis for realtime chemical sensing of PFOS and related PFAS materials. This project aims to explore this opportunity and to achieve a chemical sensor that can be used in the field without the need for sample analysis at a central laboratory. Suitable for both Honours and MRes in Chemistry.

¹ B.N. Viada, L.M. Yudi, D.W.M. Arrigan, Detection of perfluorooctane sulfonate by ion-transfer stripping voltammetry at an array of microinterfaces between two immiscible electrolyte solutions, *Analyst*, **145** (2020) 5776-5786. DOI: 10.1039/d0an00884b.

Properties and applications of ion-transfer processes at oil-water interfaces

Electrochemistry at oil-water interfaces opens up new ways to detect substances which are not easy to oxidise or reduce – it relies on ion transfer across the interface to provide an electrical current. As these electrochemical interfaces are made smaller, they are subjected to a number of changes which can improve their performances, including lower capacitances and increased diffusional fluxes.² A range of microscale and nanoscale oil-water interfaces are available to explore whether such benefits are practically useful. These interfaces can be formed at the mouths of glass micropipettes or nanopipettes, or at solid membranes containing holes punched by laser ablation or focused ion beam (FIB) milling. This project will focus on exploring the behavior of ion-transfer voltammetry at microscale or nanoscale liquid-liquid interfaces, aimed at employing this behaviour as a basis for sensitive and selective chemical detection. Specific applications can include ions of environmental or biological importance, depending on the interests of the project student.

² D.W.M. Arrigan, E. Alvarez de Eulate, Y. Liu, Electroanalytical opportunities derived from ion transfer at interfaces between immiscible electrolyte solutions, *Australian Journal of Chemistry*, **69** (2016) 1016–1032. DOI: 10.1071/CH15796.

Dr Nadim Darwish & Dr Simone Ciampi

Office: 500-4126

Lab: 500-2229

Phone: 92669792

Email: nadim.darwish@curtin.edu.au



Single-molecule Sensors

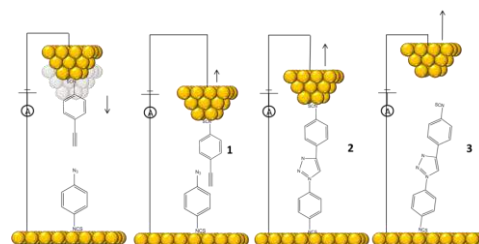
Background

Single-Molecule Electronics research combines chemistry and electronics for the aim of developing devices from single molecules. In this project, you will learn nanotechnology, electrochemistry and surface science approaches including scanning probe microscopy where you will be able to image and manipulate materials at the scale of single molecules or even individual atoms.

Honours Projects

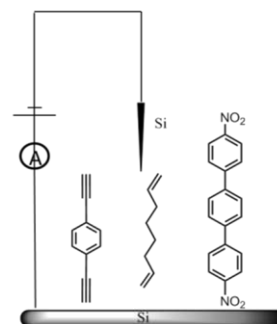
Single Molecule Reactions

Studying chemical reactions at the single-molecule level became a reality thanks to the advancement in nanotechnology. Scanning tunnelling microscopy single-molecule junctions approach is a powerful technique available for aligning and bringing together single molecule reactants between nanoscale electrodes. It has recently provided significant data^{1,2} on the variation of reaction rates and equilibria in response to external stimuli. In this project, scanning tunnelling microscopy junction approaches^{1,2} will be used to test a range of chemical reactions at the single-molecule level. This project has important implications as portable sensors with sensitivity that far exceeds any current sensing technology.



Silicon-Based Single-Molecule Circuits

The ultimate goal in molecular electronics is to use individual molecules as the robust electronic component of a real-world device. For this concept to become reality it will require the field of single molecule electronics to utilize electrode materials that are technologically relevant in the current microelectronics industry such as silicon electrodes.³ We have recently developed new methods of wiring molecules onto flat H-terminated silicon-(111) electrodes. This project aims to fabricate single-molecule contacts that mimics solid-state electronics such as diodes, resistors and transistors. This will be achieved using a modified conducting atomic force microscopy, scanning tunneling microscopy junction and mechanically controlled break junction approaches



References

1. Aragonès, A. C. *et al.* Electrostatic catalysis of a Diels–Alder reaction. *Nature* **531**, 88–91 (2016).
2. Darwish, N. A., Aragonès, A. C., Darwish, T. A., Ciampi, S. & Díez-Pérez, I. Multi-Responsive Photo- and Chemo-Electrical Single-Molecule Switches. *Nano Lett.* **14**, 7064–7070 (2014).
3. Aragonès, A. C., Darwish, N. A., Ciampi, S., J.J. Gooding, Díez-Pérez, I. Single-molecule contacts on Silicon, *Nature Communications* doi: 10.1038/ncomms15056 (2017). Media outlet- Gizmodo- *Australian scientists just made a huge breakthrough that will lead to smaller devices.*

Dr Raffaella Demichelis

Office: 500-3121

Lab: 500-1105

Phone: 9266 9027

Email: raffaella.demichelis@curtin.edu.au



Background

I develop virtual models that explain how atoms arrange into chemical structures, how molecules move and transform into one another. My team apply these methods to study how minerals grow and interact with their biological or abiotic environment. The following projects can be tuned according to the students' interest. They will improve the students' computational and physical chemistry skills, while linking these specific fields to broad interdisciplinary topics.

Exploring the biomineral/water interface (with Dr. Alicia Schuitemaker)

Living beings can grow minerals with specific shapes, textures, structures, sizes, compositions (Figure 1a-b). Calcium carbonate, phosphate, and oxalate are the most relevant minerals for humans and animals, as they build up most hard tissues and are linked to pathological conditions. To understand and learn how to prevent/promote biomineralization when needed, access to atomic scale knowledge of biomineral formation is crucial.¹

This research will focus on modelling the water/biomineral interface (e.g. Figure 1c) in presence of biomolecules_{SEP}. Outcomes will help building the puzzle of how biomolecules direct the formation of minerals.

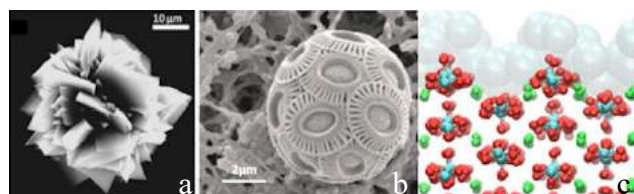
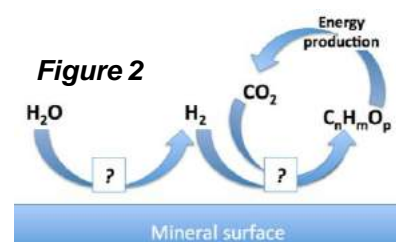


Figure 1 Biominerals from *Peperomia* sp. Leaf (a; CaC_2O_4 , Dr. H. Horner), *Emiliana huxley* (b; CaCO_3 , © The Trustees of the Natural History Museum, London). Model of a CaCO_3 surface (c; O, C, Ca, water coordination layer in red, cyan, green, transparent beads, respectively).

Structure, composition, properties and reactivity of pyroxene mineral catalyst (with Dr. Julie Aufort)

Chemical reactions occurring at the surface of minerals present in deep Earth and in space can produce organic matter from CO_2 and water,² and therefore could potentially be employed to produce clean energy according to Figure 2. However, their reaction mechanism and the catalytic role of the mineral surface are at present mostly unexplored. Pyroxene $[\text{Ca,Fe,Mg}]_2\text{Si}_2\text{O}_6$ is thought to be one of such minerals. Its cationic composition and crystal structure vary depending on the environment in which it forms. This project will employ computational tools to investigate its crystal and surface structure and composition. The main purpose of this research is to providing a realistic model that will enable future investigations on the surface reactivity of pyroxene in deep Earth and extra-terrestrial environments.



¹ Demichelis, R. et al. *Annual Review of Materials Research* **2018**, *48*, 327.

² Müntener, *Geology* **2010**, *38*, 959.

Prof. Julian Gale

Office: 500-4102

Lab: 500-4101

Phone: 9266 7800

Email: J.Gale@curtin.edu.au

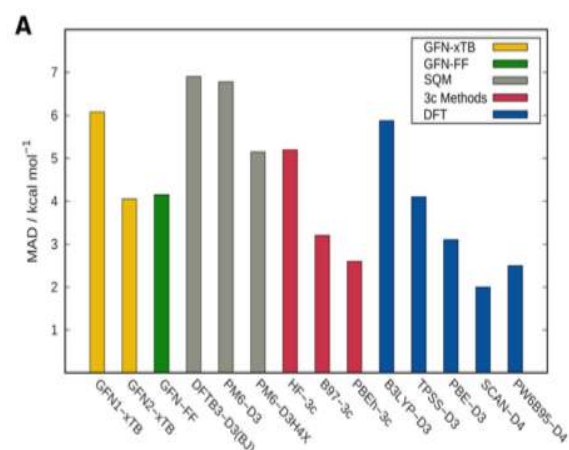


Background

My research involves the development and application of computer simulation-based techniques and theory to solve problems in the areas of chemistry, materials and geoscience. Examples of some of the research interests include crystal growth, minerals chemistry and biomineralization, solid-state materials for energy, including lithium batteries and fuel cells for hydrogen combustion, heterogeneous catalysis, nanoporous molecular sieves and membranes for desalination of water.

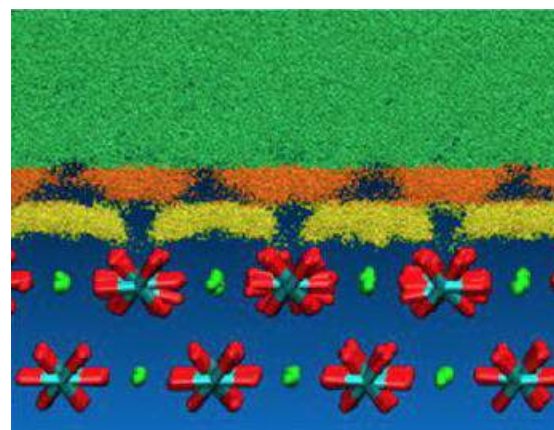
Are universal force fields universally applicable?

Force fields provide a fast approach to simulating materials properties. However, there is first the slow process of finding the parameters. The advent of so-called “universal” force fields that provide parameters for all materials without fitting avoid this barrier, but at the cost of potentially compromised accuracy. The recent GFN-FF method (S. Spicher and S. Grimme, *Angewandte Chemie Int. Ed.*, **131**, 1195 (2020)) appears to overcome this with similar Mean Average Deviations for molecules to quantum mechanical methods (see Figure). This project will test the transferability of this approach to solid materials.



Structure and stability at aqueous interfaces

The interface between a solid and solution plays a critical role in crystallization, catalysis and many other properties. In some cases, such as calcite (see Figure to the right), it is possible to resolve the structure of not only the solid at the interface, but also aqueous solution both experimentally, with X-ray reflectivity, or with computer simulation. In this project molecular dynamics simulations will be used to examine such interfaces to study the variety of different solvent structures that can be induced depend on the nature of solid and choice of surface termination.



John Curtin

Distinguished Professor

Kliti Grice

Office: 500-2116

Lab: 500-level 3

Phone: 9266 2474

Email: k.grice@curtin.edu.au



Background

My research interests are reconstructing past ecosystems and environmental changes from climate variability, molecular fossils & their individual stable C, H, S & N isotopic compositions preserved in the geological record. Some of these events are associated with mass extinction & evolution/ recovery of life (e.g. Grice et al., 2005; Tulipani et al., 2014). In addition, I am interested in studying microbial & fungal ecology, algal communities, plant physiology (including biochemical pathways) in modern environments, biogeochemical cycles (C, H, S & N) including applications of organic & stable isotope geochemistry to natural resources (petroleum & mineral geochemistry) and impacts on the environment & climate.

Role of microbial whiting events in exceptional graptolite preservation

Microbial whiting events have been observed in the Chicxulub crater and pre-Cretaceous sediments (e.g. Bralower et al., 2020; Schaefer et al., 2020) (especially those known to contain extinct graptolites) and are linked with low nutrient, alkaline water bodies dominated by cyanobacteria which can nucleate minerals around their cells initiating e.g. calcite precipitation in the water column. Such processes are probably characteristic of simple life (cyanobacteria) at the bottom of the marine food web, contributing to conditioning the oceans during the post extinction and recovery of life. The recently drilled Chicxulub crater core has recently provided the best archive of microbial changes (e.g. microbial whiting events) and the recovery of life following a major meteorite impact event at the end-Cretaceous. In extant systems, microbial whiting events can occur in alkaline, nutrient-limited lakes. Lake Walyungup in Western Australia is a modern day (Holocene) system known to contain a whiting event. The lake will be cored and compared with ancient fossilized and extinct graptolites to help elucidate the molecular composition of microbial whiting events in modern and deep-time samples. The student will also investigate nucleation processes of modern insects containing chitin (cf. graptolite's exoskeleton) in microbial mats mesocosms to uncover past fossilisation/preservation processes.

Molecules of life in fossilized cells from fish in the Santana Formation

Concretions are often preserved in sediments and can contain encapsulated fossil remains (e.g., bones, plants and insects). Concretions formed under highly reduced conditions allow for exceptional preservation of soft tissue, cells and biomolecules (e.g., sterols and proteins) (Melendez et al., 2013a, 2013b; Plet et al., 2017). Concretions therefore represent molecular time capsules that may contain evidence of species that evolved or became extinct. With access to concretions from various worldwide locations (e.g., Cretaceous Santana Formation, Brazil) the project will involve detailed state-of-the art isotopic, geochemical, analytical, mineralogical and imaging techniques of a unique fossil (fish and scales) inside a concretion. The intact molecules will be extracted and analysed to provide important paleoenvironmental information on the lipid preservation in the Cretaceous fish.

Dr Hendra Gunosewoyo

Office: 306-103

Lab: 306-117

Phone: 9266 3747

Email: Hendra.Gunosewoyo@curtin.edu.au

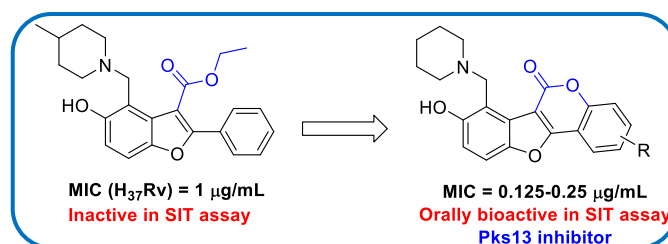
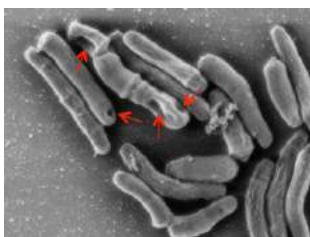


Background

Research in my group is largely based around the rational design and synthesis of small organic molecules to combat infectious diseases and inflammatory disorders. We utilise modern synthetic medicinal chemistry techniques to create novel molecules with unique modes of action that effectively target the infectious agents of interest. The current disease focus is on tuberculosis with collaboration partners in the Center for Tuberculosis Research, Johns Hopkins University, USA. We are also expanding our medicinal chemistry capabilities to synthetic cannabimimetics, aiming for potent and selective cannabinoid type 2 (CB₂) receptor agonists as well as brain-penetrant kinase inhibitors. Both projects offered below will be done in collaboration with Dr Alan Payne and A/Prof Mauro Mocerino.

Molecular Interventions for Tuberculosis

Mycolic acids are integral constituents of the unique, thick lipid-rich cell wall of *Mycobacterium tuberculosis* (*M.tb*). The project aims to develop small molecules capable of inhibiting the transport of essential mycolic acid across the cell wall of *M.tb*. Our group discovered the indoleamides as a novel chemical entity from high throughput screening and elucidated its mechanism of action via whole genome sequencing, namely via inhibition of Mycobacterial membrane protein large 3; MmpL3 [1]. More recently, we are also working on small molecule inhibitors of Pks13, another crucial enzyme involved in the biosynthesis of mycolic acids [2].



Deciphering Coconut Oil Constituents for Neonatal Sepsis

The group at KEMH has previously shown that topical administration of coconut oil to preterm infants drastically improved their underdeveloped skin without adverse side effects [3-5]. It is now known that monolaurin, the major constituent in coconut oil, is the key component that has been tested as a single agent for the antimicrobial effects. This project aims to further extend our understanding on what other ingredients in coconut oil may be responsible for the skin protective effects. We seek to build a body of structure-activity relationship data on existing and novel fatty acid derivatives, particularly looking at the antimicrobial and wound-healing properties. Final compounds will be tested for their in vitro efficacies in collaboration with Prof. Tobias Strunk and Telethon Kids Institute.

[1] Lun, et al. (2013) Indoleamides are Active Against Drug-Resistant *Mycobacterium tuberculosis*. *Nature Comm.* 4: 2907.

[2] Zhang et al. (2018) Identification of Novel Coumestan Derivatives as Polyketide Synthase 13 Inhibitors against *Mycobacterium tuberculosis*. *J. Med. Chem.* 61: 791-803.

[3] Molloy, E. J., et al. (2020) Neonatal sepsis: need for consensus definition, collaboration and core outcomes. *Pediatr Res* 88(1): 2-4.

[4] Strunk, T., et al. (2019) Routine Use of Topical Coconut Oil in Extremely Preterm Infants. *Neonatology* 115(4): 346-347.

[5] Strunk, T., et al. (2019) Topical Coconut Oil Contributes to Systemic Monolaurin Levels in Very Preterm Infants. *Neonatology* 116(3): 299-301.

Dr Mark Hackett

Office: 500-4125

Lab: 500-Level 3

Phone: 9266 3102

Email: mark.j.hackett@curtin.edu.au



Background

I am an analytical chemist and my research interest is the development and optimization of novel elemental and bio-molecular imaging techniques, which are applied across the biological sciences. The spectroscopic techniques involved in my research program include Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy, X-ray fluorescence spectroscopy (XRF), and X-ray absorption spectroscopy (XAS). These techniques can be used to image: lipid and protein oxidation products (FTIR and Raman); biochemical markers of altered metabolism (FTIR); hemoglobin oxygenation (Raman); elemental distribution (XRF); transition metal oxidation state (XAS); sulfur oxidation state (XAS). I primarily use these techniques to understand brain chemistry, in both normal and diseased brain function. The methods also find use in the environmental sciences, for example, detecting microplastics in environmental samples. As a student in my group you will gain a fundamental understanding of applied spectroscopic analysis of biological systems, and excellent technical training on operation of state-of-art spectroscopy instruments and software programs used for data analysis.

Honours Projects

“Lipids and Brain Disease” (with Associate Professor Ryu Takechi and Professor John Mamo, CHIRI): My research group has recently identified biomarkers of altered lipid homeostasis during accelerated ageing, which may contribute to dementia in the elderly. Using several spectroscopic modalities (FTIR, Raman, UV-VIS), this project will extend from the preliminary data, and characterise spectroscopic bio-markers of lipid oxidation, in order to monitor the role of lipids, lipid metabolites and lipid oxidation products in brain disease. This project has scope to be performed in collaboration with the Curtin Health Innovation Research Institute, and would be very well suited to an aspiring chemist with interests in the biological or health sciences.

Microplastic detection: The natural environment is under a deluge from plastic contamination. It is becoming increasingly important to identify and characterize the abundance and type of microplastics found in environmental systems (e.g., water, soil, organisms). Vibrational spectroscopy techniques such as FTIR and Raman have strong potential for use in this research area. In the project you will investigate, develop and optimize analytical protocols through which micro-plastic contamination in the environment can be studied.

Dr Guohua Jia

Office: 500-3119

Lab: 500-2222

Phone: 9266 7882

Email: guohua.jia@curtin.edu.au



Background

One-dimensional (1D) metal halide perovskite nanorods are emerging as a type of materials with remarkable optical and electronic properties such as linearly polarized light emission, reduced lasing threshold and improved charge transport. These properties make them stand out from perovskite nanocrystals of other morphologies in a variety of applications such as liquid crystal displays (LCDs), light-emitting diodes (LEDs), photodetectors, solar cells and photocatalysis. Research into this field is rapidly expanding and growing in the past several years, with significant advances in both mechanistic studies of their growth and widespread applications.

The fascinating and useful applications of perovskite nanorods such as CsPbX_3 ($X=\text{Cl, Br}$ and I) are underpinned by the high quality nanomaterials with controlled size, shape and composition and good stability for practical use under hard conditions. Although there are a few documented attempts for the controlled chemical growth of perovskite nanorods, research into this area is still in its infancy. Due to ionic nature of the metal halide crystal lattices, chemical reactions of the synthesis are extremely fast, making it challenging to gain high-degree of control of perovskite nanorods in terms of size, aspect ratio and performance. Furthermore, because of the ionic nature of metal halide perovskite nanorods, they are a bit sensitive to moisture and may undergo decomposition at elevated temperatures. Therefore, it is highly demanded to develop facile, robust and scalable synthetic approaches for the preparation of high-quality perovskite nanorods, to enrich the existing knowledge of their growth mechanisms, and to improve their stability that underpins their future applications.

Colloidal One-Dimensional Metal Halide Perovskite Nanocrystals for Optoelectronic Devices

This project aims to design and controllably synthesize a family of metal halide perovskite CsPbX_3 nanorods with desirable optical and electronic properties using chemical synthetic routes. Specifically, we aim

- (1) Use systematic, integrated, multidisciplinary approaches to the design and synthesis of perovskite CsPbX_3 nanorods with controllable size, aspect ratios and composition.
- (2) Develop strategies to increase the stability of the perovskite CsPbX_3 nanorods by reducing the growth rates and surface defects and by overgrowing a passivating layer of materials.
- (3) Investigate the photoluminescence anisotropy of single perovskite CsPbX_3 nanorods, and develop alignment approaches appropriate for elongated CsPbX_3 nanorods to construct polarized light-emitting diodes (LEDs) for solid-state lighting.
- (4) Fabricate perovskite CsPbX_3 nanorods-based photovoltaic devices and optimise their performance in terms of durability and energy efficiency.

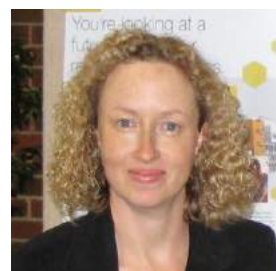
Prof. Cynthia Joll

Office: 500-3117

Lab: 500-3222, 3225, 3227

Phone: 9266 7229

Email: c.joll@curtin.edu.au



Background

My research interests are focused on water chemistry, e.g. drinking water quality and treatment and wastewater treatment for the purposes of water recycling, and environmental chemistry.

Improving Drinking Water Treatment Processes (with Dr Ina Kristiana (Curtin Chemistry); WA Water Corporation and other industry partners)

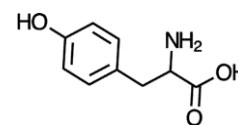
Natural organic matter (NOM) is a complex matrix of simple and macromolecular organic molecules originating from the decomposition of plant and animal materials in natural systems. NOM in drinking water source waters is a major problem in drinking water treatment. Every form of chemical disinfection reacts in some way with NOM, producing undesirable disinfection by-products (DBPs). Some of these DBPs have recommended guideline levels due to long-term public health risks. In this project, you will investigate adsorption methods for improved NOM removal in drinking water treatment processes, in collaboration with industry partners. The efficiency of these adsorption methods will be evaluated in laboratory studies by their removal of NOM, bromide and DBP precursor compounds.

The Evolution of Drinking Water Treatment in WA: Effect on Disinfection By-Products (with Dr Yolanta Gruchlik (Curtin Chemistry); WA Water Corporation)

Disinfection of drinking water is essential for public health protection, however, unintended chemical disinfection by-products (DBPs) are produced during drinking water treatment via reactions between the disinfectant (e.g. chlorine) and natural organic matter (NOM) and/or bromide which is naturally occurring in some source waters. More than 600 DBPs have been identified in drinking water, and many of them are potentially mutagenic or carcinogenic. Climate change in WA has led to an evolution in drinking water supplies and treatment technologies. In this project, you will investigate the effect of some of these changes on the formation of DBPs in the drinking water distribution system. Using sample preconcentration equipment, GC-MS instrumentation and a state-of-the-art halogen-specific total organic halogen analyser, your project will contribute to a better understanding of DBPs currently formed in WA distribution systems.

Mechanism of Formation of a Key Nitrogenous Disinfection By-Product (with Dr Ina Kristiana (Curtin Chemistry) and Dr Kathryn Linge (ChemCentre))

Nitrogenous disinfection by-products (N-DBPs) can form when dissolved organic nitrogen reacts with disinfectants such as chlorine or monochloramine. We have previously investigated the formation of one commonly detected N-DBP, dichloroacetonitrile (DCAN), from the reaction of monochloramine with model nitrogen-containing compounds. We identified a new pathway for DCAN formation from cleavage of activated aromatic structures after electrophilic substitution of chlorine and addition of monochloramine to the ring system. This project will study an expanded range of model compounds, including relevant biomolecules, to confirm the link between activated aromatic compounds and DCAN formation during chloramination, and perform experiments to further understand the formation mechanism. You will use electron ionization (EI) GC-MS to study fragmentation patterns and by-products, and stable isotopes (e.g. ^{15}N and ^{13}C) to elucidate formation mechanisms.



Dr Franca Jones

Office: 500-4121

Lab: 500-2242

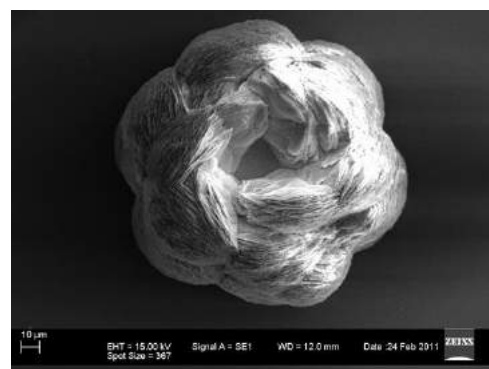
Phone: 9266 7677

Email: F.Jones@curtin.edu.au



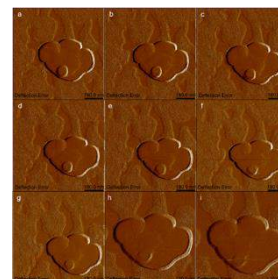
Background

Crystallization is an important field both from a fundamental and an applied perspective. One aspect in particular that permeates my research is the role of impurities on the crystallization of inorganic and organic species. These projects have broad applications to real life; from understanding how crystals grow in nature to how they grow inside humans! All projects will involve learning a variety of techniques (e.g. Infrared, Raman, AFM, batch morphology experiments, analytical techniques) and developing your problem solving skills. Projects can be somewhat adjusted to suit a particular interest.



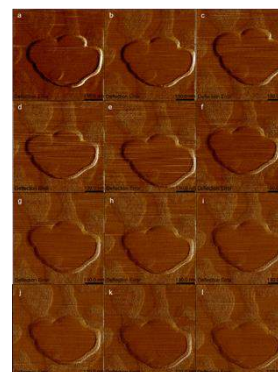
***In-situ* investigation of clay dissolution (collaborators include Tom Becker, Peter Smith, Jose Gomez)**

Clays in bauxite have the possibility of dissolving and contributing to desilication products and scale formation in the Bayer process (process to refine bauxite to alumina). Despite this, very little is known about how these clays behave in high caustic environments. This project is an extension of work completed on kaolinite in caustic whereby other, different clays known to be found in bauxite are investigated using Atomic Force Microscopy.



New additives for scale inhibition (collaborators include: Mark Ogden, Peter Roth, George Shimazu, Tom Becker)

This project is about understanding the role of inhibitors and their impact on crystallization modification. Various additives (small molecules and polymers) will be used to determine the impact on various salts that are known scale compounds and the mechanism of interaction through small batch crystallization methods including DLS and conductivity but may move onto more sophisticated methods such as AFM and infrared.



Dr Peter Kraus

Office: 500-4112

Lab: 500-1105

Phone: 9266 3730

Email: peter.kraus@curtin.edu.au



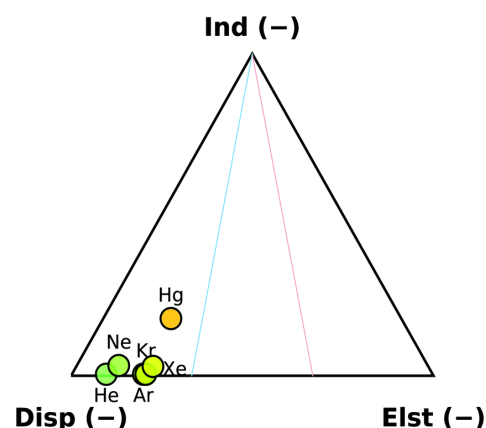
Background

My research focuses on the application of quantum chemistry to predict structures of molecules, model chemically relevant processes, and investigate properties of materials. I am interested in supporting and complementing experimental research: accurate prediction of structures informs characterisation using spectroscopic methods; determining accurate reaction rates allows chemical engineers to optimize engines and reactors.

Trends in structures of van der Waals complexes of noble gases and CO₂

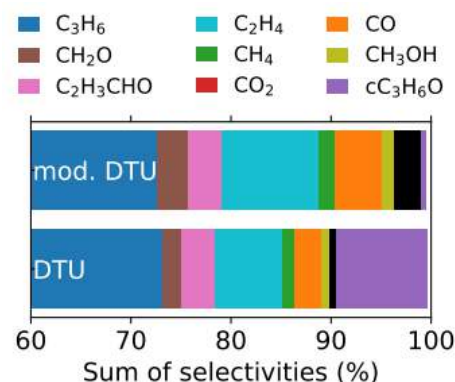
(with J/Prof. Dan Obenchain, University of Göttingen) We have previously shown that the complexes of He, Ne, Ar, Kr, Xe, and Hg with OCS follow clear trends in structure due to the stabilising electrostatic interaction (elst) due to the increased polarisability of the rare gas atom, with the Hg complex being the clear outlier with a significant induction (ind) component. We could also show the importance of relativistic effects for predicting the structure of Xe...OCS. The complexes of the same elements with CO₂ have been studied using microwave spectroscopy. The goal of the project is to investigate the trends in structure and binding of the CO₂ and see whether comparisons with the OCS series can be made.

We have previously shown that the complexes of He, Ne, Ar, Kr, Xe, and Hg with OCS follow clear trends in structure due to the stabilising electrostatic interaction (elst) due to the increased polarisability of the rare gas atom, with the Hg complex being the clear outlier with a significant induction (ind) component. We could also show the importance of relativistic effects for predicting the structure of Xe...OCS. The complexes of the same elements with CO₂ have been studied using microwave spectroscopy. The goal of the project is to investigate the trends in structure and binding of the CO₂ and see whether comparisons with the OCS series can be made.



Decomposition pathways of propylene oxide from first principles

A revised combustion mechanism for propane has been recently published by researchers at the Technical University of Denmark (DTU). This mechanism is significantly more accurate at predicting various properties of low-temperature and high-pressure propane flames. However, in a recent study we could show that under certain conditions propylene oxide (cC₃H₆O) forms a mechanistic “dead end”. This is not surprising, as the formation pathways of cC₃H₆O are included, but its decomposition is not. Modification of the DTU mechanism (mod. DTU) is necessary to align the model with the observed behaviour. This project will involve using state of the art computational methods to predict the kinetics of cC₃H₆O decomposition, and validation of these new pathways against literature combustion and catalytic data.



Prof. Simon Lewis

Office: 500-2117

Lab: 500-3229

Phone: 9266 2484

Email: s.lewis@curtin.edu.au

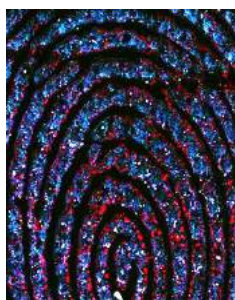


Background

My research interests are focused upon analytical chemistry techniques applied to forensic science, with a particular focus on exchange evidence. Areas of specific interest include: the characterization and interpretation of chemical trace evidence, latent finger mark chemistry and the detection of latent finger marks. Projects in the areas below can be tailored to meet the interests of students.

Detection of latent fingermarks (with Dr Georgina Sauzier and Prof Bill van Bronswijk)

Successful development of latent fingermarks relies heavily upon the chemistry of the latent finger mark residue and of the substrate upon which the mark is deposited. Research at Curtin has in recent years investigated a range of approaches to the detection of latent fingermarks on a range of surfaces including gold nanoparticles¹ and near infrared luminescent pigments². We have also been investigating the fundamental chemical and physical properties of latent fingermark residue^{3,4}. This research will be carried out with input from the Western Australia Police Forensic Division.



Analysis and interpretation of chemical trace evidence (with Dr Georgina Sauzier and Prof Bill van Bronswijk)

There is an increasing demand for scientifically rigorous approaches to the analysis and interpretation of forensic evidence. Over the last few years our group has been collaborating with ChemCentre, the forensic chemistry service provider in Western Australia, on a range of projects relating to the analysis and interpretation of physical evidence. This has included automotive paint⁵, explosives⁶ and most recently soil⁷. Many of these projects have made use of chemometrics, which can ensure quantitative, objective measures of a dataset are obtained; thereby improving reliability, reproducibility and discrimination of the data, whilst simultaneously addressing issues concerning observer bias and other sources of human error in forensic examinations. This project will be carried out in close collaboration with ChemCentre.



1. T.G. Newland, S. Moret, A. Bécue and S.W. Lewis, *Forensic Science International*, 2016, **268**, 62-72.
2. B. Errington, G. Lawson, S. W. Lewis, and G.D. Smith, *Dyes and Pigments*, 2016, **132**, 310-115.
3. B.N. Dorakumbura, R. E. Boseley, T. Becker, D. E. Martin, A. Richter, M. J. Tobin, W. Van Bronswijk, J. Vongsvivut, M. J. Hackett, and S. W. Lewis, *Analyst*, 2018, **143**, 4027-4039
4. R.E. Boseley, B. N. Dorakumbura, D. L. Howard, M. D. De Jonge, M. J. Tobin, J. Vongsvivut, T. T. M. Ho, W. Van Bronswijk, M. J. Hackett, and S. W. Lewis, *Analytical Chemistry*, 2019, **91**, 10622-10630
5. K. van der Pal, G. Sauzier, M. Maric, W. van Bronswijk, K. Pitts, and S. W. Lewis, 2016, *Talanta*, **148**, 715-720
6. H.A. Yu, D. A. DeTata, S. W. Lewis, and N. Nic Daeid, 2017, *Talanta*, **164**, 716-726
7. H.A. Yu, N. Nic Daeid, L. A. Dawson, D. A. DeTata, and S. W. Lewis. 2017, *Plos ONE*, **12**, e0189177. <https://doi.org/10.1371/journal.pone.0189177>

Prof. Andrew B. Lowe

Office: 500-2151

Phone: 9266 9281

Email: andrew.b.lowe@curtin.edu.au



Background

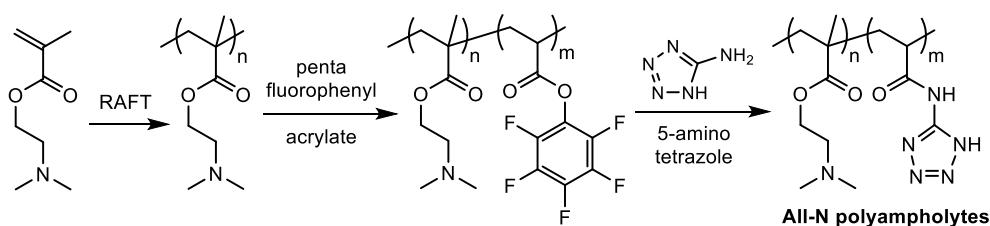
We are a synthetic polymer group with interests spanning radical and metal-mediated controlled polymerizations such as reversible addition fragmentation-chain transfer (RAFT) polymerization and Rh-mediated insertion processes, stimulus responsive ('smart') polymers, and polymer-related 'click' chemistries.

Tetrazole: A Carboxylic Acid Bioisostere and the Synthesis of Polymeric Protein Mimics

Tetrazoles are nitrogen-based heterocycles with many interesting properties. However, the tetrazole functional group is largely unexplored in synthetic polymer chemistry despite its properties and potential applications of molecules containing such functionality. One particularly important feature of

tetrazoles is their ability to serve as chemical mimics of carboxylic acids. In the field of medicinal chemistry such functional groups

are referred to as bioisosteres. This project will focus on the synthesis of a new family of protein-mimetic polymers known as polyampholytes,^[1-3] see Scheme; these are polymers that contain, or potentially contain, anionic and cationic charge with the former most commonly being a carboxylic acid. This project will prepare and characterize a new family of such materials based on all-nitrogen building blocks in which the carboxylic acid functionality is replaced with a tetrazole.



Organic-Inorganic Polymer-based Hybrid Materials with Potential as Bioimaging Agents (Lowe & Massi)

Recently we have been examining the synthesis and photophysical properties of polymers containing luminescent rhenium-based fragments.^[4-6] We have shown that the hybrid materials retain the desirable photophysical properties of the rhenium fragment after complexation to the polymer backbone. This project builds on our initial studies and aims to prepare new multifunctional hybrid materials containing luminescent rhenium and iridium fragments. The project will utilize the RAFT-polymerisation technique to prepare reactive precursor copolymers based on poly(ethylene glycol) and pentafluorophenyl acrylate followed by chemical modification with various amines and finally attachment of the rhenium and iridium fragments. The project involves a combination of synthesis and characterization including photophysical studies. Participants will receive training in advanced polymer synthesis and modification, NMR spectroscopy, including the use of ¹⁹F NMR as a reaction monitoring tool, size exclusion chromatography (SEC) and fluorimetry as a tool to examine the photophysical properties of the hybrid materials.

[1] Lowe et al. *Macromolecules* **1998**, *31*, 5991; [2] Lowe and McCormick *Chem. Rev.* **2002**, *102*, 4177; [3] Wang and Lowe *J. Polym. Sci., Part A: Polym. Chem.* **2007**, *45*, 2468; [4] Dallerba, Massi, Lowe *Eur. Polym. J.* **2020**, *126*, 109559; [5] Dallerba, Massi, Lowe *Polymer* **2020**, *128*, 109559; [6] Fantini et al. *Macromol. Chem. Phys.* **2020**, *221*, 202000135.

Prof. Ricardo L. Mancera

Office: 305-161

Lab: 305-154

Phone: 9266 1017

Email: R.Mancera@curtin.edu.au

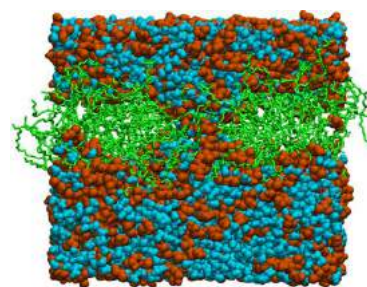


Background

My research in biophysical chemistry uses computational and biophysical methods such as molecular dynamics simulation, molecular modelling, structural bioinformatics, surface plasmon resonance, X-ray scattering and thermometric methods. We investigate biomolecular structure, function and interactions, such as protein folding and aggregation, cell membrane stability, the self-assembly of macromolecular complexes, drug-protein / protein-protein / protein-DNA interactions, drug delivery across membranes, and molecular forces in aqueous systems.

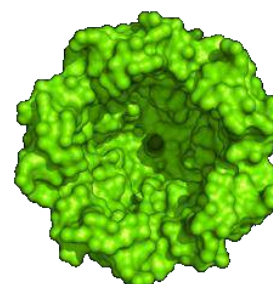
Effect of cryosolvents on the structure and stability of model cell membranes

Cryopreservation (the storage of cell and tissues at liquid nitrogen temperatures: -196°C) requires the use of so-called cryosolvents to promote the vitrification of water inside cells to minimize ice formation. Cryosolvents such as DMSO and glycerol are toxic to cells and can damage cell membranes by changing their structure and functionality. In this project molecular dynamics simulations will be used to predict changes in the structure and stability of model cell membranes at various levels of hydration in the presence of aqueous solutions of cryosolvents. This will allow the rational design of optimal mixtures of cryosolvents for improved cryopreservation of germplasm, eggs and embryos.



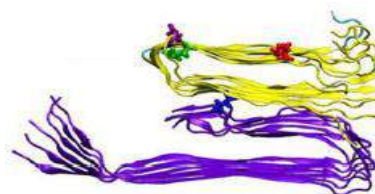
Molecular structure and stability of proto-cells

Primordial cells are believed to have combined primitive nucleic acids and polypeptides within a self-assembled protective membrane made up of amphiphilic molecules. This project will use molecular dynamics simulations to characterise the structure and formation of model proto-cells by describing the self-assembly of lipid vesicles made of simple fatty acids around macromolecular complexes made of peptides and nucleic acids. Understanding the molecular forces responsible for the formation of proto-cells and the influence of high temperature and salt concentration will shed light on the likely chemical evolution pathways on early Earth.



Are diabetes and Alzheimer's disease linked? Biophysical studies of the aggregation of amyloidogenic proteins.

Type-2 diabetes (T2D) increases the risk of Alzheimer's disease (AD). The underlying molecular mechanism remains unknown but is probably mediated by the accumulation and cross-aggregation of amyloid beta ($\text{A}\beta$) and amylin (normally found in the pancreas) in the brain. Cross-aggregates of these proteins have been shown in vitro to be toxic to brain cells. This project will use circular dichroism, infrared spectroscopy and surface plasmon resonance to measure the kinetics and affinity of binding of $\text{A}\beta$ and amylin. The outcomes will shed light into the cross-seeding mechanism behind the synergistic interaction of these two proteins, which could be targeted with anti-aggregation drug molecules to reduce neuronal cell death in AD.



A/Prof. Max Massi

Office: 500-3118

Lab: 500-2219

Phone: 9266 2838

Email: m.massi@curtin.edu.au

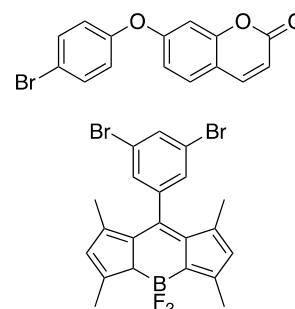


Background

The research in our group is centred on the design, synthesis and application of luminescent organic molecules and metal complexes, with an emphasis of assessing them as tools for diagnostic imaging and potential new therapeutic agents. Projects encompass a mixture of synthetic chemistry, photophysical characterisation and application of the prepared compounds in the field of life science. These can be tailored according to your preference, so the description provided below are just for a general idea.

Discovering new molecular tools for imaging the neurochemistry of brain disease (with Dr Mark Hackett)

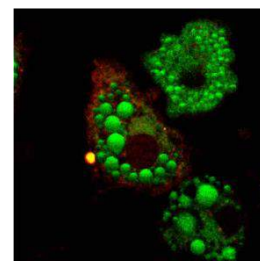
There is currently substantial research effort being directed to identify the chemical pathways through which neurodegeneration and neurological disorders manifest and progress. Understanding the neurochemical pathways of brain disease will then help drive rationale therapy development, which could have substantial human health and economic benefits. State-of-the-art microscopy techniques allow imaging of cells and tissue with subcellular resolution. This project will focus on synthesising and testing new luminescent molecules, such as those shown in the figure, that can be exploited for the imaging of brain tissue.



The research will be multidisciplinary at the boundary of synthetic chemistry and life science.

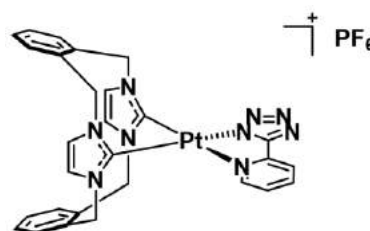
The molecular approach to discover biochemical processes in live cells

The direct optical visualisation of lipids and lipid trafficking in live cells is challenging due to the drawbacks associated to the currently available markers for lipids. In our studies, we have discovered some unusual molecular species containing metals such as rhenium and iridium that are not only able to localise with polar lipids in cells, but they are also able to track their “movement” between cell compartments. These new tools are proving very valuable to develop new molecular probes and associated protocols for various diseases, and to directly investigate their biochemical progress in cells. In this project, you will design, synthesis and investigate new luminescent species for the study of biological processes and the diagnosis of various pathologies including cancers.



Can metal complexes aid in the search of new antibiotics?

The scientific community is currently struggling to keep up with the pace at which bacterial infections are evading antibiotics through the development of multidrug resistance. We have recently discovered a Pt complex (shown in the figure) that displays antibacterial and antifungal properties while showing low toxicity to mammalian cells. By synthesising analogous species, this project will seek to investigate whether the structural features of this compound can assist in the discovery of new antibiotics.



Prof. Mark Ogden

Office: 500-2114

Lab: 500-2219

Phone: 9266 7265

Email: m.ogden@curtin.edu.au



Background

Research in the group is currently focused predominantly on lanthanoid coordination chemistry (with some involvement of *d*-block complexes). The lanthanoids lurk at the bottom of the Periodic Table and are sometimes forgotten, despite the fact that they are vital for many technologies (for example, your smart phone most likely contains at least six different lanthanoids). The lanthanoids have important magnetic and light-emitting properties. Our program of research is focused on understanding how lanthanoid complexes emit light – we want to make materials that do this more efficiently, and we can only do that if we understand the underlying processes. To do this, we need to control the coordination chemistry of these fascinating metal ions.

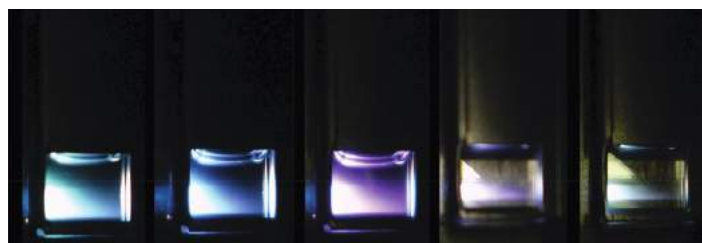
Honours Projects

Lanthanoid Complexes for Light Emitting Materials (with Max Massi, Mauro Mocerino)

Lanthanum 57 La 138.91	Cerium 58 Ce 140.12	Praseodymium 59 Pr 140.91	Neodymium 60 Nd 144.24	Promethium 61 Pm [144.91]	Samarium 62 Sm 150.36(2)	Europium 63 Eu 151.96	Gadolinium 64 Gd 157.25(3)	Terbium 65 Tb 158.93	Dysprosium 66 Dy 162.50	Holmium 67 Ho 164.93	Erbium 68 Er 167.26	Thulium 69 Tm 168.93	Ytterbium 70 Yb 173.05	Lutetium 71 Lu 174.97
--	-------------------------------------	---	--	---	--	---------------------------------------	--	--------------------------------------	---	--------------------------------------	-------------------------------------	--------------------------------------	--	---------------------------------------

Lanthanoids have fascinating magnetic and light-emitting properties that lead to a range of current and potential applications. Despite all the research to date, some aspects of their behaviour are still not well understood. For example, while the processes taking place in systems that emit visible light have been made quite clear, emission in the near infrared is still something of a mystery that we are trying to solve. This project will require you to:

- Synthesize known and new ligands and/or *d*-block metal complexes, that can act as an antenna for near infrared emitting systems, or form complexes with specific coordination geometries. Possible antenna systems include β -diketonates, calixarenes, and rhenium or ruthenium complexes.
- Synthesize and characterize lanthanoid complexes or polymetallic assemblies.
- Study the photophysical properties of the resulting materials.
- Use these results to design more efficient light emitting systems.



Dr Alan Payne

Office: 500-4120

Lab: 500-2229

Phone: 9266 1917

Email: alan.payne@curtin.edu.au



Background

My research interests lie in organic synthesis, with an emphasis on biologically relevant molecules. I am also interested in the interactions of small organic molecules in biology for drug discovery and the agricultural industry. The projects offered will give you experience in a broad range of synthetic organic chemistry to solve problems at the biology-chemistry interface.

Honours Projects

Plant growth regulators and unusual molecules

Plant growth regulators are important in all facets of agriculture from increased production, reducing wastage to herbicides. Surprisingly, these regulators are simple molecules (e.g. ethylene) and their derivatives can be accessed simply through synthesis. The aim of the project will be to *make and test* interesting molecules that act as either agonists or antagonists of these regulators. The picture to the right shows the protective effect of an ethylene antagonist toward flower drop caused by ethylene.

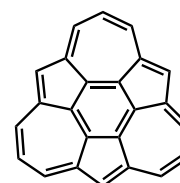


Natural products of native Western Australian plants

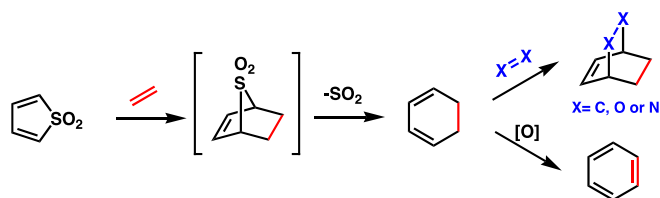
The resinous coating of many Australian plants contains interesting compounds. This project will isolate and identify compounds, such as clerodanes, from the resinous coating of plants. Their chemistry will then be investigated concentrating on abundant compounds with could be used as scaffolds in the pharmaceutical industry.

Exotic Molecules

There are many unusual or exotic molecules that have been overlooked by the chemical community. Some of these molecules probe our fundamental understanding of chemical principles and others are useful in making medicinally relevant molecules. Isocoronene (right) and 1,2,3-triazaazulene are molecules that have yet to be made with potentially interesting properties. Another exotic molecule is thiophene-1,1-dioxide which can be used to make medicinally useful



Isocoronene



Diels-Alder reaction of thiophene-1,1-dioxide

compounds. It reacts as a diene in the Diels-Alder reaction (left). After a cycloaddition event, the resultant adduct spontaneously loses sulfur dioxide to generate a new diene, which can either react further in another cycloaddition event or be aromatised to a benzene derivative.

A/Prof. Paolo Raiteri

Office: 500-4122

Lab: 500-1105

Phone: 9266 2687

Email: p.raiteri@curtin.edu.au

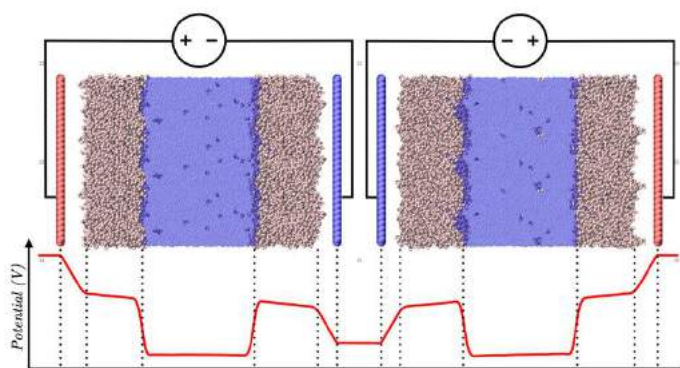


Background

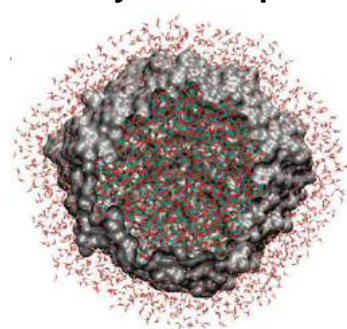
My research focuses on the development and application of computational techniques to study technologic and fundamental problems in the areas of chemistry, physics and geoscience. I am especially interested in studying the thermodynamics and kinetic aspects of the problems. Examples of my research interests include crystal growth, mineral chemistry and bio-mineralization.

Atomistic structure of the interface between two immiscible liquids

Solid-solid interfaces have been extensively studied and a lot is known about their mechanical and electronic properties, particularly for semiconductor materials. However, much less are known about liquid-liquid interfaces. This not due to a lack of scientific interest or importance, but because the ever-changing arrangement of the atoms at the interface between two fluids makes it almost impossible to build any simple models that can be used to predict the properties of the interface. Due to the high mobility of the molecules the interface between two immiscible liquids is not sharp and fluctuates in time, which greatly reduces the ability of most experimental techniques employing light scattering or atomic force microscopy to identify the structure at the boundary. Here computer simulations can offer a unique insight into the molecular structure of the interface by providing an atomically resolved picture of the two fluids.



Stability of amorphous minerals in aqueous environment



Minerals are ubiquitous materials that are relevant for many industrial and biological processes. The very existence of many marine organisms and vertebrates animals indeed heavily depends on the use of bio-minerals for protection (exoskeleton), movement (bones), feeding (teeth) and even orientation. Calcium carbonate is one of the most common bio-minerals and there is growing evidence that it is often stored in hydrated amorphous nanoparticles prior to its utilization. Amorphous materials are extremely difficult to characterize because of their intrinsic disorder and even more so at the nanoscale, which is beyond the resolution limit of many experimental techniques.

Computer simulations therefore have the unique opportunity to provide atomistic insight into the structural and dynamical properties of these materials and assist with the interpretation of the experimental data.

A/Prof. Debbie S. Silvester

Office: 500-3120

Lab: 500-2222

Phone: 9266 7148

Email: d.silvester-dean@curtin.edu.au

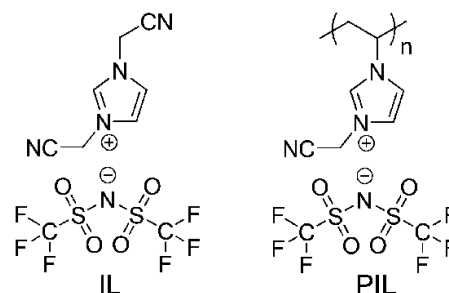


Background

My research lies at the boundaries of physical, analytical and materials chemistry. My group uses sophisticated electrochemical techniques to detect species such as toxic gases and explosives dissolved in liquid samples. We employ room temperature ionic liquids (RTILs) as electrolytes/solvents due to their highly favourable properties, such as non-volatility, intrinsic conductivity, high chemical stability, wide electrochemical windows and the ability to dissolve a wide range of compounds (and generally because we think they're great).

Electrochemical Sensing of Gases in Real Environments using Ionic Liquids and Poly(Ionic Liquids)

Gas sensors are important tools that enable the identification and quantification of individual gases, and identify leaks to prevent harmful effects on people and the environment. Amperometric gas sensor (AGS) research has recently been moving towards miniaturised designs, with the removal of the gas-permeable membrane, and the application RTILs or 'gelled' RTILs as non-volatile and robust electrolytes. In this project, you will work towards understanding the behaviour of gases in ionic liquids and poly-ionic liquids (PILs) with a view to develop highly robust sensors. The information uncovered will help towards the development of sensors for gases based on gelled ionic liquid electrolytes. This work could lead to exciting collaborative opportunities with a gas sensor company in Switzerland, who are working with us to develop a new generation of sensors based on these exciting materials.



Detection of explosives on different surfaces for forensic swabbing applications

Explosive compounds are widely used in demolition, mining, and for military purposes. Their reduction products can be toxic and carcinogenic to humans, and may contaminate drinking water. Due to a range of security and environmental needs, the development of sensors for explosives is of huge interest. Various techniques have been developed to detect explosives, with electrochemical methods offering advantages of low-cost instrumentation, portability, durability, sensitivity, and rapid response times.



In this project, you will work towards the development of a swabbing electrochemical device for picking up trace amounts of explosive material from different surfaces. We have already demonstrated that a poly-ionic liquid (PIL, see figure above) can be used as both a collection and detection material for solid TNT on aluminium foil. This project would expand that work, by investigating different explosive compounds, such as DNT, RDX and HMX, and also different surfaces, including clothing, plastic, glass and other surfaces where explosive residues may be present. The results from this project will provide important information on the viability of electrochemical sensing systems for detecting trace explosives on complex surfaces.

A/Prof. Daniel Southam

Office: 500-3116

Phone: 9266 2380

Email: d.southam@curtin.edu.au



Background

Chemistry Education is my area of research interest. My broad aim is to improve students' perceptions and to develop capacity for real change in the depth of their understanding and enjoyment of Chemistry. This year's projects are just suggested topics, and students who have a particular direction within these broad ideas will be given autonomy to direct the project to match their interests.

Disruptive or disrupted — what is the role of chemists and chemistry in the 21st century?

Technology-led disruption of the workforce is a pressing issue for future employability, with up to 40% of the Australian workforce at significant risk of automation or mechanisation in the next 20 years.³ Therefore, we must empower the next generation of chemistry graduates with an ability to identify opportunities for advancement of the profession. To achieve this requires a curriculum that supports the knowledge, skills and literacies to enable full participation in the future global workforce. This project will focus on the identifying the skills and knowledge in the chemical sciences that are required for future employment. We will chart the development of these skills throughout the curriculum and develop and evaluate the efficacy of modules designed to build them in a chemistry context.

Motivation and meaningful learning in chemistry

The primary learning environment in our first-year chemistry units at Curtin is a workshop, where students work together on activities, small assessment tasks, and present their findings to the class. The workshop environment is intended to foster positive student motivation toward meaningful learning. We know a little bit about student attitudes and self-efficacy in this environment,⁴ but not much about how their motivational status might be supported and developed. This project will study students' individual motivational statuses using two different models of motivation⁵ and link these to meaningful learning⁶ of chemistry concepts. The outcomes of this project will help us understand how we might support students' motivations, and how this may be developed as a consequence of learning experiences.

³ CEDA. *Australia's future workforce?* Melbourne, Australia: Committee for Economic Development of Australia; 2015 May. Frey CB, Osborne MA. *The Future of Employment: How susceptible are jobs to computerisation?* Oxford Martin School; 2013 Sep.

⁴ Xu X, Alhooshani K, Southam D, Lewis JE. Gathering Psychometric Evidence for ASCIv2 to Support Cross-Cultural Attitudinal Studies for College Chemistry Programs. In: Kahveci M, Orgill M, editors. *Affective Dimensions in Chemistry Education*. Berlin, Heidelberg: Springer Berlin Heidelberg; 2014. pp. 177–94. Vishnumolakala VR, Southam DC, Treagust DF, Mocerino M, Qureshi S. Students' attitudes, self-efficacy and experiences in a modified process-oriented guided inquiry learning undergraduate chemistry classroom. *Chem Educ Res Pract*. 2017;18(2):340–52.

⁵ Liu Y, Ferrell B, Barbera J, Lewis JE. Development and evaluation of a chemistry-specific version of the academic motivation scale (AMS-Chemistry). *Chem Educ Res Pract*. 2017;18(1):191–213. Gegenfurtner A, Hagenauer G. Achievement goals and achievement goal orientations in education. *International Journal of Educational Research*. 2013;61:1–4.

⁶ Novak JD. Meaningful learning: The essential factor for conceptual change in limited or inappropriate propositional hierarchies leading to empowerment of learners. *Science education*; 2002;86(4):548–71.

Prof. Raphael A. Viscarra Rossel

Office: 500-4114

Lab: 500-Level 2

Phone: 9266 1154

Email: r.viscarra-rossel@curtin.edu.au



Background

We conduct theoretical, methodological and applied research to improve understanding of soil processes and the drivers of soil and landscape variability at different spatial and temporal scales. Our research aims to quantify, assess and monitor soil functions, which help to deliver ecosystem services that enable life on Earth. The research that we do can help to: create sustainable landscapes and ecosystems, ensure sustainable food, fiber, water and energy production, improve nutrient management, monitor and verify soil carbon (C) sequestration, improve and rehabilitate degraded land, rehabilitate contaminated soil, mitigate climate change.

Characterising the mineral and organic composition of rangeland soils with FT-IR spectroscopy. Supervisors: R. Viscarra Rossel & Pogs Manalili. FT-IR spectra of soil are full of information on the soil's inherent composition: its minerals and organic matter. The project aims to develop a spectroscopic method for cost-efficient estimation of soil properties in dryland environments, using these spectra. Activities: laboratory measurements of soil with a FT-IR spectrometer and statistical multivariate modelling. Suited to students who are interested in a combination of laboratory and statistical modelling.

Fractionating soils to characterise their mineral-organic composition. Supervisors: R. Viscarra Rossel & Pogs Manalili. Soil organic carbon is important for soil health, productivity and potentially, can also help to mitigate climate change. Understanding its composition is important. This project will develop a method to fractionate soils to derive different soil organic carbon fractions with different organic-mineral properties and turnovers. Activities: intensive mostly laboratory-based research with some statistical data analysis. Suited to students who are interested in laboratory method development.

Characterising the spatial-temporal variation of soil respiration under cropping and native pastures. Supervisors: R. Viscarra Rossel. An improved understanding of temporal and spatial variations in soil respiration is essential for accurately measuring soil CO₂ efflux and for assessing ecosystem carbon budget. This project will analyse respiration under different land uses. Activities: field measurements of soil respiration and geostatistical analyses. Suited to students who are interested in a combination of field work and spatial modelling.