





2021 HONOURS/MASTERS RESEARCH PROJECTS

DEPARTMENT OF CHEMISTRY & PHYSICS





CONTENTS

Honours / Masters Courses	1
Chemistry Research	6
Physics / Nanotechnology Research	9
Chemistry Projects	
Masters of Chemical Science – Research Skills Project	14
Belinda Abbott - Medicinal Chemistry	16
Carmel Abrahams - Supramolecular Chemistry	18
Peter Barnard - Organic and Inorganic Synthetic Chemistry	19
Jason Dutton - Synthetic Main Group Chemistry	21
Conor Hogan - Electrochemistry, Photochemistry and Sensors	23
Yuning Hong – Materials and Biological Chemistry	25
Adam Mechler - Biophysical Chemistry and Nanochemistry	27
Nick Reynolds – Self-Assembling Nanomaterials	29
Evan Robertson - Optical Spectroscopy	31
Pallavi Sharma – Synthetic Organic Chemistry	33
Brian Smith - Modelling Molecular Interactions	34
David Wilson - Computational Chemistry	36
Physics Projects	
Brian Abbey - Advanced Molecular Imaging	38
Narelle Brack - Nano-structured Materials, Interfaces & Surface Science	40
David Hoxley – Low-dimensional Electronics and biosensing	42
Shanshan Kou – Biophotonics	44
Chris Pakes - Nanophysics and Atom-scale Research	46
Paul Pigram - Nano-structured Materials, Interfaces and Surface Science	48
Chanh Tran - X-ray Physics	51
Grant van Riessen - X-ray Microscopy and Condensed Matter	53
Projects Selection Form	56

HONOURS/MASTERS COURSES

Why do Honours or Masters?

Honours/Masters in chemistry or physics is a great way to kick-start your career in science. The Honours/Masters research program equips graduates with technical, analytical, communication and time management skills demanded by employers in diverse scientific fields. An Honours/Masters degree also adds a new dimension to the skills acquired during your undergraduate studies; it provides students with their 'first taste' of research. Students have the opportunity to join a research team and contribute to original research at the cutting edge of science, with personal mentoring from an expert academic in a research project of your choice. Honours/Masters provides training in research techniques and skills plus experience with contemporary research. Our students have access to some of the best research facilities in the world, in the \$100M La Trobe Institute for Molecular Science (LIMS).









Objectives

- · Extend students' depth and breadth of knowledge in their discipline
- · Provide experience in different laboratory practices
- · Plan and carry out experimental procedures
- · Pursue an original research project

Skills

- · Apply a range of practical and analytical techniques required for research
- Develop effective time management skills
- · Read and understand the technical literature, interpret results and critically evaluate published data
- · Develop communication skills required to present to a scientific audience
- · Work independently and as part of a research group

COURSES AND CORDINATORS

Honours in Chemistry Dr Pallavi Sharma

Master of Chemical Science Dr Peter Barnard

Honours in PhysicsDr Grant van RiessenMaster of NanotechnologyDr Grant van RiessenMaster of Science in Physical ScienceDr Grant van Riessen

COURSE STRUCTURE

The course extends beyond the standard undergraduate semesters, which reflects the transition from undergraduate student to graduate researcher.

February, 2021 and conclude in early November. The program starts with a series of compulsory induction lectures. The assessment will vary slightly depending on your course but in general the first assessment is a literature review related to the project that students are undertaking. The majority of the year is dedicated to conducting research, which culminates in writing a final research thesis. During the year you will learn about what it takes to be an expert researcher across a set of diverse research topics by attending the weekly department research seminars. Students will give an initial presentation of their research plans in May and a final seminar in late September, where students' research findings for the year are presented. Students complete their research in early October, after which they focus on writing their thesis to be submitted in late October. The year culminates in an oral examination of the thesis in early November. Supervisors will continuously assess students' research performance throughout the year.

Throughout the year you will develop individual investigative skills, critical thinking and the ability to analyse experimental data. You will learn to evaluate scientific and professional literature, to articulate your knowledge and understanding in written and oral presentations, and to work as part of a team.

What does it lead to?

An Honours/Masters degree significantly enhances your career prospects and provides a pathway to a postgraduate degree (PhD) with a supported scholarship. An Honours/Masters degree is a necessary requirement for proceeding to further research work, either in industry, a research institution such as CSIRO, or a university. Most employers give preference to Honours/Masters graduates, particularly for the more interesting, non-routine jobs. Even in employment areas that do not utilise the specific scientific content, such as the Public Service, value research training.

ELIGIBILITY, ENTRY REQUIREMENTS AND HOW TO APPLY FOR HONOURS/MASTERS PROJECTS

Entry Requirements

Entry requirements for Honours are:

- Completion of an undergraduate degree, and
- An average grade of at least 65% in 60 credit points of third year of your major, and
- An overall third-year average (120 credit points total) of at least 60%, and
- Agreement of a supervisor

Note that all four requirements must be met for acceptance into Honours.

Masters of Chemical Science research year:

- An individual academic supervised research project requires an average grade of at least 65% in 60 credit points of CHE3 subjects (4 subjects), and agreement of a supervisor.
- The Research Skills Project provides training in a range of chemistry research skills.
 All students can select this project however students who do not obtain the 65% average will undertake this project. Each project stream incorporates equivalent learning outcomes and assessment and provides the opportunity to apply for entry into a PhD program.
- Mid-year entry is available for Honours in Chemistry and for Masters of Chemical Science.

Application Process

- 1. Both Honours and Masters Students must complete the Project Preference form on the last page of this booklet and submit it by the date provided on the form.
- 2. Honours students must also formally apply through Apply Online from the University website). If you are unsure about this process, contact ASK La Trobe. As soon as examination results are available, all students who qualify for entry to Honours in Chemistry will be notified by email and provided with further information about re-enrolment and the structure of the Honours year. Any student who does not receive a letter but believes they are eligible should contact the Honours Coordinator.

Students from other institutions

Applications from students at institutions other than La Trobe are welcome, for which equivalent grades will be required for entry. A student must have completed all the requirements for a pass degree before enrolment in Honours is permitted.

SELECTING A SUPERVISOR AND PROJECT



Choosing a supervisor and project is a very important aspect of undertaking Honours/Masters research. You should give careful consideration to selecting a supervisor and a project, with both aspects being equally important. Firstly, you should choose an area of chemistry or physics that you are interested in, however it is important to retain a broad interest and an open mind

about potential supervisors and projects. You should also consider the track record and experience of the supervisor. It is useful to speak to current Honours, Masters and PhD students about their experiences and the projects they are working on.

Research topic: What area of chemistry or physics do you find interesting? To what extent will the background knowledge and understanding from your undergraduate studies prepare you for each of the research topics? Be open-minded about projects, as you will learn very useful skills in any project.

Supervisor: Does the supervisor have a track record of supervising students and producing research outcomes (journal publications, patents)? What style of supervision do you prefer? How does the supervisor provide feedback on presentations and thesis drafts? Does the supervisor have the funds to support the project?

Career opportunities: How will the project complement your chosen career, including possible postgraduate research (if applicable)?

It is essential that you discuss projects with prospective supervisors. Don't be afraid to ask! You can only answer these questions by talking to prospective supervisors. Supervisors are generally very keen to discuss their research. A summary of the current research activities of the Chemistry and Physics academics are described in this booklet. In considering these offerings, students are advised to maintain a broad range of interests, to consider projects in both chemistry and physics, and are encouraged to discuss all of the projects that appeal to them with the members of staff concerned.



As part of the project selection process, students are asked to nominate at least THREE choices (and preferably more) of research supervisors in order of preference (see final page of this booklet) and must obtain the signature of the supervisor as proof that the student has discussed the project.

CHEMISTRY AND PHYSICS

Please note that no commitments regarding allocation to a particular project or particular supervisor can be made at the initial stage of discussions with potential supervisors, as all offers of project places are subject to approval by the Head of Department.

Projects are also frequently offered that are partly or wholly off campus in collaboration with external bodies such as the Environmental Protection Agency (EPA), the Department of Primary Industries (DPI), The Walter and Eliza Hall Institute of Medical Research (WEHI), CSIRO, Victoria Police Forensics Department and other universities.

Masters of Chemical Science students: The research year achieves the equivalent of the Honours year. There are two streams of the research year, with entry into the research group stream requiring a higher level of performance in the first year of the course. The Research Skills Project is broad-based and available to all students.

Masters of Nanotechnology and Physical Science students: The research year achieves the equivalent of the Honours year. There are two streams of the research year, with entry into the research group stream requiring a higher level of performance in the first year of the course.

Students are encouraged to consider the projects based in both Physics and Chemistry disciplines. Interdisciplinary projects co-supervised by other departments are an option.

Masters students complete a project in their second year, for which the application process is the same as for Honours. Masters students must nominate at least THREE (and preferably FOUR or more) research supervisors, and must obtain the signature of the supervisor as proof that the student has discussed the project with the supervisor.

PROJECT ALLOCATION PROCESS

Projects are allocated to students based on student preferences (using the form at the back of this project booklet), student marks and availability of places in research groups. Students will also be distributed across research groups (using student preferences) to maximise the ratio of supervisor to student to ensure personal mentoring of students. If multiple students have the same preference for supervisor, then students will be ranked on the basis of their marks.



Once subject results are available from the previous semester, students who qualify for entry to Honours or Masters projects will be notified by email about their nominated project, with details on enrolment requirements and commencement dates.

CHEMISTRY AND PHYSICS

DEPARTMENT OF CHEMISTRY AND PHYSICS

The Department of Chemistry and Physics, including research laboratories, teaching facilities and administration is housed in the LIMS1, LIMS2 and PS1 buildings. These buildings contain 10,000 sq m of usable space including 18 new research and support laboratories, an equipment barn, a 200-seat auditorium and approximately 3000 sq m of teaching facilities.

The Department of Chemistry and Physics is part of the School of Molecular Sciences and the La Trobe Institute for Molecular Science (LIMS).

Research within LIMS is aimed at generating **Translatable Molecular Discoveries** and encompasses **research within four themes**:

Cancer

Infection and Immunity

Nanoscience

Molecular Design

The majority of chemistry and physics research is carried out within the last two themes.

CHEMISTRY

Chemistry has a rich history of excellent research. Professor Jim Morrison AO (who the first-year chemistry prize is named after) is widely regarded as the father of mass spectrometry in Australia. Such research excellence has attracted exceptional researchers to come here, including Professor John Fenn (Nobel Prize winner 2002) who worked in Chemistry as a Distinguished Visiting Scientist. Dr Maureen Mackay, the first female academic in chemistry at La Trobe, worked with Dorothy Hodgkin (Nobel Prize 1964) to solve the structure of Vitamin B12.

Chemistry has now entered an exciting new era as part of the **La Trobe Institute for Molecular Science (LIMS)** including brand new and purpose-built research laboratories. Academics in Chemistry carry out cutting edge research across all areas of modern chemistry, from synthesis through modelling and physical chemistry to chemical analysis and nanotechnology.

Chemistry offers a world-class research environment for training and conducting research, highlighted by the recent visit of Noble Laureate Prof Barry Sharpless in 2018.

Our graduates are in high demand from employers. Many of our PhD students have received acknowledgements and awards for their research. Our honours graduates are highly sought after, with many having been awarded Australian Research Scholarships and are currently undertaking PhDs in the Department and elsewhere.



Examples of previous graduates include:

- Dr Terri Field-Theodore received her PhD in 2019 and is now a Postdoctoral Research Fellow at Tianjin University, China.
- Kaitlyn Cullum completed Honours in 2018 and is now employed as a Chemist at Advanced Molecular Technologies, Melbourne.
- Will Graf completed Honours in 2018 and is now employed at the Police Forensics Laboratory.
- Dr Luke Duncan received his PhD in 2017 and is now a Postdoctoral Researcher at Bayer Crop Science.
- Dr Melissa Buskes received her PhD in 2016 and is now an Associate Research Scientist at Northeastern University, USA.
- Dr Brad Sleebs received his PhD in 2004 and is now a senior researcher at the Walter and Eliza Hall Institute (WEHI) in medicinal chemistry.
- Dr Ellen Reid received her PhD in 2012 and is now working as a Patent Scientist at JonesTulloch.
- Professor David Craik received his PhD in 1981 and is now a leader in NMR and biomolecular structure within IMB at the University of Queensland.

CHEMISTRY RESEARCH FACILITIES

Chemistry has moved into the new LIMS building, a state-of-the-art facility with 10,000 sq m of usable space including 18 new research and support laboratories, an equipment barn, a 200-seat auditorium and about 3000 sq m of teaching facilities.

Current equipment includes:

- 400 and 500 MHz NMR instruments.
- IR / UV-Visible Spectrometers
- Mass Spectrometers
- Single crystal X-ray diffraction
- HPLC
- Atomic force microscope and fluorescent microscope
- · Raman and IR microscopes
- Thermogravimetric analyser
- Specialist synthesis facilities
- Access to HPC supercomputers





PHYSICS AND NANOTECHNOLOGY

We offer a dynamic Honours/Masters program linked to our research specialisations in the areas of functional materials and surface physics, nanophysics, and X-ray physics. Honours/Masters attend advanced lecture courses and seminars.

An Honours or Masters degree may lead to the opportunity to proceed to a postgraduate degree such as a PhD in Physics, with financial support from a postgraduate scholarship. An Honours or Masters degree also provides a gateway to careers in research physics, either in industry, or research organisations such as CSIRO, DST Group and universities. It will also provide distinctive opportunities in applied physics such as medical physics and geophysics.



An Honours/Masters degree in Physics or Nanotechnology is highly regarded by prospective employers. It extends the range of employment possibilities to areas such as quantitative analytics for the finance sector. Even in employment areas that do not utilise the specific scientific content, such as the Public Service, the value of the research training is nevertheless recognised. All eligible students should give serious consideration to undertaking the Honours/Masters year.

Many of our PhD students have received acknowledgements and awards for their research. Mark Edmonds was awarded the Australian Institute of Physics Thomas H Laby Medal for the most outstanding Honours physics thesis in Victoria followed by an Australian Synchrotron Postgraduate Award. In 2011 Corey Putkunz won the Australian Synchrotron Thesis Medal.

We frequently offer projects that are partly or wholly based off- campus in collaboration with external organisations such as the Australian National Fabrication Facility, the Australian Synchrotron, CSIRO, DST Group and other universities.

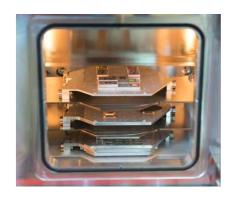
CHEMISTRY AND PHYSICS

Examples of previous graduates include:

- Dr Nicholas Philips received his PhD in 2018 and is now a Scientist at the Department of Engineering Science, University of Oxford.
- Dr Henry Kirkwood received his PhD in 2017 and is now a Scientist at the European XFEL in Germany.
- Dr Corey Putkunz received his PhD in 2011 and is now a Geophysical Software Developer at Downunder GeoSolutions based in Western Australia.
- Dr Andrew Walter received his PhD in 2011 and is now a Scientist at Brookhaven National Laboratory in the USA.
- Dr Anton Tadich received his PhD in 2008 and is now a Scientist at the Australian Synchrotron in Melbourne.
- Professor Catherine Stampfl received her PhD in in 1990 and is now a leader in condensed matter physics at the University of Sydney.

Study options

Research training in Physics and Nanotechnology is offered to students at all post-graduate levels. Honours and Masters students who enter the research stream in their second year undertake four advanced courses (15 credit points each) and undertake a major research project (60 credit points) hosted by one of our research laboratories.



Students should discuss projects with potential supervisors, who will assess an interested student's ability to undertake a particular research project in their area of research and give feedback to the student regarding their capacity to supervise the project. Students need to submit their project preferences to the Physics Postgraduate Coordinator before enrolling in the appropriate thesis subjects.

Nanotechnology students can pursue Honours or Masters projects in fields relating to their major studies, for example physics, chemistry, biochemistry and mathematics. Nanotechnology students are encouraged to consider physics projects and interdisciplinary projects co-supervised by staff in collaborating disciplines and departments.

RESEARCH in PHYSICS and NANOTECHNOLOGY

Research in Physics is broadly defined by two themes: functional materials and surface science, and X-ray science. The Department hosts the Centre for Materials and Surface Science and a node of the ARC Centre of Excellence for Advanced Molecular Imaging. We also have strong links to internationally recognised research facilities including the Australian Synchrotron, the Australian National Fabrication Facility, the Melbourne Centre for Nanofabrication, and links to research organisations such as CSIRO and the DST Group. Strong focus is placed on Condensed Matter Physics and Optical Physics, which are both fields in which La Trobe University received the highest rating ('well above world standard') during the Excellence in Research for Australia (ERA) national research assessment.

Functional materials and surface science

The research groups of Brack, Hoxley, Pakes and Pigram make up this theme, which is primarily concerned with fundamental electronic properties of emerging materials, the fabrication and characterisation of technologically important surfaces and nanomaterials, and their application in the fields of quantum devices, biosensing, drug delivery, advanced materials and minerals.

X-ray science

The research groups of Abbey, Nugent, Tran and Van Riessen make up this theme, which is primarily concerned with the coherent properties of X-rays, the interaction of X-rays with matter and their application to imaging and structure determination using a range of local and international synchrotron, laboratory-based, and free-electron laser X-ray sources.



PHYSICS AND NANOTECHNOLOGY RESEARCH FACILITIES

Our Melbourne-based laboratories house an extensive range of instrumentation including:

- X-ray photoelectron spectroscopy
- Time of flight secondary ion mass spectrometry
- Auger spectroscopy
- Ultra-high vacuum instruments for low-temperature scanning tunnelling microscopy
- Versatile scanning probe microscopy
- Facilities for material processing and nanofabrication
- X-ray microscopy and microtomography
- Coherent (lensless) optical imaging
- High-performance computing and visualisation tools
- A dedicated helium liquefier for low-temperature techniques
- Astronomical telescopes

Other facilities include access to La Trobe Microscopy resources including electron microscopy, light and confocal microscopes, and analytical X-ray facilities. We also make extensive use of major research facilities such as the Australian Synchrotron and the Melbourne Centre for Nanofabrication.

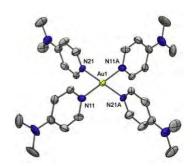
The Physics discipline interacts strongly with synchrotron radiation facilities around the world. We lead internationally recognised research in the fields of coherent X-ray science and experimental condensed matter physics. We have developed major synchrotron instrumentation that has been deployed at the BESSY synchrotron (Berlin), the Advanced Photon Source (Chicago) and the Australian Synchrotron (Melbourne). Currently we operate three instruments at the Australian Synchrotron: a custom-built Angle-resolved Photoemission Spectrometer, a state-of-the-art X-ray detector and a soft X-ray nanoscope for which a dedicated branch beamline was constructed. Physics also established Australia's first remote access 'Virtual Beamline' – a computerised Visualisation Laboratory providing global research opportunities for postgraduate students and staff.

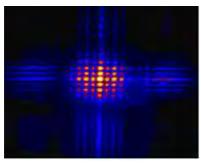
Our research groups have an excellent track record of being granted access to major neutron, synchrotron radiation and X-ray free electron laser facilities. Our researchers were the first Australian group to be awarded access to the most powerful X-ray laser in the world.

2021 RESEARCH PROJECTS IN CHEMISTRY, PHYSICS AND NANOTECHNOLOGY

A summary of the current research activities of the Chemistry and Physics academics are described in this booklet. See each member of staff in the following pages for more details.

Students will need to discuss projects with potential supervisors. In considering these offerings, students are advised to maintain a broad range of interests in their discipline and even across disciplines, and are encouraged to discuss all of the projects that appeal to them with the members of staff concerned.







CHEMISTRY PROJECTS



Masters of Chemical Science

Research Skills Project

The Research Skills Project is designed as an alternative pathway for the second (research) year of the Masters of Chemical Science program. The second year usually involves students choosing a supervisor and conducting a year-long research project in the supervisor's laboratory. The research year provides students with a high level of indepth training in one specific area of chemistry e.g. synthetic chemistry, computational chemistry or analytical chemistry and is assessed via a literature review, seminar and the final research thesis and oral examination.

In contrast, the Research Skills Project is tailored to give students research training in a variety of different chemistry disciplines and consists of an integrated series of five smaller projects. The projects run one after the other and will enable you to focus on one specific area of chemistry at a time.

A range of projects will be offered and these will change from year to year. Examples of projects are: computational chemistry, analytical chemistry, and organometallic synthetic chemistry. The computational project will provide you with training in how computational methods can be used help researchers understand the structure and reactivity of molecules, while in the organometallic synthetic chemistry project you will study how metal-based catalysts can be prepared and used in the synthesis of organic molecules such as medicines. Each project will be a supervised by a member of academic staff from Chemistry in addition to an expert demonstrator, who will help you conduct the experimental



work. You will meet with the project supervisor each week to prepare a project plan and to discuss your research results. The experimental laboratory work will be undertaken two days per week, with the remainder each week being dedicated to experimental design and analysis of results.

The Research Skills Project will be assessed in the same way as the individual research project. For each of the five research skills included you will prepare a short literature review for the research field and a thesis chapter, which will include your literature review and describes your research results. Over the course of the year you will produce five chapters for the five research projects you undertake, these will be combined to produce



a final Masters of Chemical Science thesis that will be assessed at the end of the project year. You will also give a seminar at the same time as the other Master of Chemical Sciences students. The research skill project has equivalent learning outcomes and assessment to the research project and provides the opportunity to subsequently apply for PhD scholarships.

The Research Skills Program is an exciting alternative pathway that will build on your undergraduate studies and the Masters of Chemical Science coursework and will develop a range of skills and expertise that provides the basis for further studies and employment.

The Research Skills Program is available to all Master of Chemical Sciences students. Students who pass the first year of coursework but do not obtain an average grade of at least 65% in 60 credit points of CHE3 subjects (4 subjects) will undertake the Research Skills Program.

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Medicinal Chemistry

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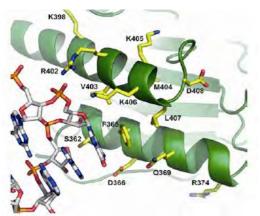


LIMS Theme: Molecular Design Positions available: One

Medicinal chemistry involves the design, synthesis and development of the molecules we need in order to understand, prevent and treat disease. Research projects in medicinal chemistry primarily use the practical skills required for synthetic organic chemistry including techniques such as NMR, HPLC and MS. Biological assays allow the study of the structure-activity relationships of the compounds against the target.

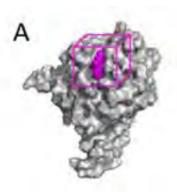
Exploring FBDD to interrupt bacterial signaling between SRP and FtsY

The bacterial signal recognition particle (SRP) is an essential ribonucleoprotein complex responsible for the delivery of membrane and secretory proteins to the plasma membrane in bacteria. Interrupting the interactions of SRP with the SRP receptor (FtsY) represents a promising strategy for the development of novel antibiotics. This project aims to expand fragments obtained from a screening library into higher affinity



compounds using the approach of fragment-based drug design (FBDD).

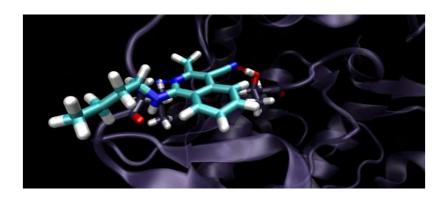
Design, synthesis and evaluation of Drp1 inhibitors

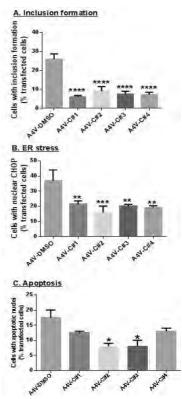


The mitochondrial protein dynamin-related protein (A) has been implicated in the development of a number of neurodegenerative diseases, including Alzheimer's disease. To date, no direct small molecule inhibitors of human Drp1 have been identified. This project aims to develop small molecules that can potently and selectively inhibit human Drp1 to provide important research tools to reveal the specific role of Drp1 in dementia and as potential leads for drug development.

Inhibiting P.falciparum in the search for a new antimalarial agent

Malaria has a significant impact on the health and economy of the developing world. Enzymes, which are important in the life cycle of the malaria parasite, could possibly be attractive targets for novel antimalarial agents. We are synthesising analogues of the isoquinoline compound A4 (shown) to evaluate against *Plasmodium falciparum* in order to develop a selective and potent inhibitor.





Targeting Rab1 for the effective treatment of motor neurone disease (MND)

Rab1 has a significant role in protein transport in cells. Transport is necessary to supply a motor neuron with components necessary for its maintenance and survival, and to remove waste products. We have identified a compound that enhances Rab1 activity and decreases ER stress, prevents the formation of inclusions and prevents apoptosis (cell death). We seek to develop compounds with this neuroprotective activity, similar to Rab1 expression, as there is currently no effective therapeutic treatment for MND.



Dr Carmel ABRAHAMS

Supramolecular Chemistry

Senior Lecturer

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LIMS Theme: Molecular Design **Positions available:** None in 2021

Supramolecular Chemistry

Crystalline coordination polymers with well-defined pores (as indicated in figure 1) may be generated by the combination of metal ions with bridging ligands. Through appropriate choice of metal ions and ligands it is possible to tailor these materials for specific uses such as the separation or capture and storage of small molecules which occupy intraframework voids. ln this project the student will synthesise and structurally characterise novel materials that are able to serve as host networks. The student will also investigate the adsorption properties of these materials.

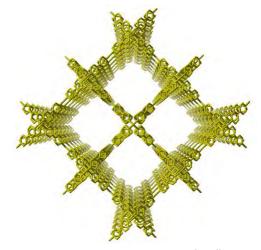


Figure 1: Single network of [Cu^ICu^{II}(bpy)₄]³⁺

Dr Peter BARNARD

Organic and Inorganic Chemistry

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LIMS Theme: Molecular Design Positions available: Two

The synthesis and development of organic ligands and coordination complexes for medicinal and biological imaging applications is the focus of the Barnard research lab. Organic and inorganic synthetic chemistry in combination with a wide range of analytical techniques are used for the generation and characterisation of new compounds.

(1) Synthesis and Studies of Luminescent Ruthenium, Iridium and Lanthanide Complexes

New luminescent and electrochemiluminescent coordination compounds of ruthenium, iridium and the lanthanide metals including *d-f* heterobimetallic arrays are being developed for potential bioimaging and sensor applications. (For some recent articles on this work see: R. E. Karmis et al. Dalton Transactions, **2019**, 48, 9998-10010; L. M. Quan, et al., Journal of Inorganic Biochemistry, **2020**, 206, 111047.)

(2) New antibiotic silver and gold N-heterocyclic carbene complexes

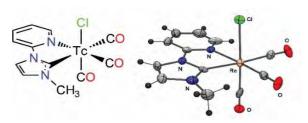
Antimicrobial coinage metal (Cu, Ag and Au) complexes of N-heterocyclic carbene ligands are under development. Recently a series of heterobimetallic Au-Ag complexes and homobimetallic Ag₂, Au₂ complexes were evaluated against clinically relevant bacterial strains and these compounds

showed broad-spectrum antibacterial activity. In this project you will prepare and evaluate new potent antibacterial compounds. T. P. Pell eta al. Inorganic Chemistry, 2016, 55, 6882-6891. IF = 4.85, C = 25

(3) Radiopharmaceutical Imaging Agents for Cancer Diagnosis

This is a collaborative project with the Australian Nuclear Science and Technology Organisation (ANSTO) involving the development of new radiopharmaceutical imaging agents for disease diagnosis. A range of ligand systems are being used in combination

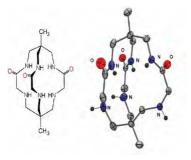
with metallic radionuclides such as Tc-99m, Cu-64 and Zr-89. Technetium-99m is the most widely used radionuclide in medical imaging and a wide array of ^{99m}Tc labelled compounds are used to image different organs and a



number of diseases. As all isotopes of Tc are radioactive, we develop new chemistry using Re and we have prepared a series of Re(I) complexes of NHC ligands. Recently we have also labelled these NHC ligands with ^{99m}Tc. See: *Chemical Communications* 53 (15), 2311-2314, **2017** and *Inorganic chemistry* 53 (20), 10862-10873, **2014**.

(4) Synthesis and coordination chemistry of amide containing molecules

The amide or peptide functional group is critical to life as it provides the linkage between adjacent amino acid residues proteins. **Amides** also interesting in display coordination chemistry, where the nitrogen atom deprotonate and coordinate to a metal ion. We are working on the synthesis of new ligands incorporating amide groups. The picture shows a triamidetriamine macrobicyclic cage ligand designed to form highly stable metal complexes. See: Tan, K. et al. Organometallics **2013**, 32, (6), 1913-1923.





Barnard research group 2019

Dr Jason DUTTON

Inorganic Chemistry

Associate Professor, ARC Future Fellow

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LIMS Theme: Molecular Design Positions available: Two

The Dutton research group is interested in fundamental studies into new structure and bonding for the elements contained within the p-block and d-block. We are currently working on a number of projects within this broad scope; projects of particular interest available for honours studies are detailed below.

Project #1: Catalysis using a new family of highly charged gold compounds We have discovered a new family of gold compounds – Au(III) trications bound by only monodentate ligands. These molecules are completely unprecedented, which offers an excellent opportunity to discover new gold based chemistry. This project will entail reacting the Au(III) trications with a variety of organic (i.e. alkynes) and inorganic (i.e. H_2 , H_2O) molecules in the hopes that new catalytic transformations can be uncovered. Ultimately this very exploratory (read as fun!) project will give an indication of the possible chemistry associated with the Au(III) trications, allowing for more targeted investigations towards the end of the project.

Project #2: Predicting new molecules (with Dr Wilson)

Doing chemistry in a computer has many practical advantages over chemistry performed on the bench. Many more "reactions" can be probed and no waste is generated. Potentially highly toxic, explosive or otherwise unstable molecules can also be explored in perfect safety. J. Dutton and D. Wilson have identified many s-, d- and p-block projects of interest. In line with the interests of a student choosing this project, an appropriate system will be explored. This will consist of searching for stable new compounds using our chemical intuition, then examining the bonding and potential properties of the molecules *in silico*.

A student joining the Dutton research group can expect to become proficient in:

- 1. A variety of inorganic (and some organic) synthetic techniques, including performing chemistry under an inert atmosphere using Schlenk and glovebox techniques.
- 2. Analyzing new compounds using multinuclear NMR spectroscopy, as well as vibrational spectroscopy and mass spectrometry.
- 3. Growing single crystals of new compounds for X-ray diffraction studies. Interested students may also be introduced to the solving and refining of their own X-ray diffraction data.
- 4. Learning the basics of performing theoretical chemistry using the Gaussian program in order to predict molecular properties. Of course, a student taking on project #2 would become advanced in this area.



Dutton lab

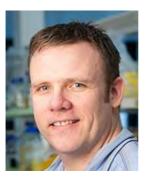
Dr Conor HOGAN

Analytical Chemistry, Electrochemistry, Luminescence and Sensing Technology

Associate Professor

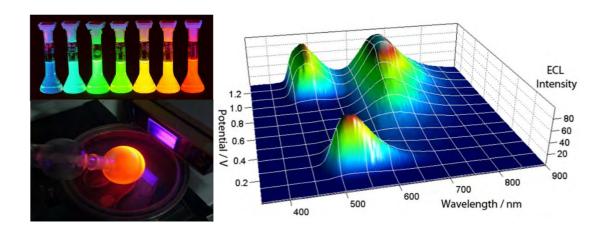
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LIMS Theme: Nanoscience Positions available: Two

Research in our group is focused on expanding the bounds of Analytical Chemistry. We seek to develop new chemistries and new technologies, which will result in exquisitely low detection limits, enhanced selectivity and miniaturised instruments that can be used in the real world outside of the laboratory setting.



Synthesis, photophysics and electrochemistry of highly luminescent transition metal complexes

We are interested in developing and investigating materials which are electroactive, materials which are luminescent and in particular, materials which have both of these properties simultaneously. For example, one area of interest is in the synthesis and applications of highly luminescent Iridium and ruthenium complexes (with Dr Barnard). We explore the use of such molecules for applications in ultra-sensitive medical diagnostic and health testing applications.

Android Voltammetry: A simple but powerful smartphone-based biosensing platform

The development of simple, inexpensive (yet quantitative) sensors for environmental,



medical and other sensing applications is an extremely important emerging area because it has the potential make (bio)chemical analysis, usually confined to the lab, more widely available. Such technology would be transformational, particularly in remote areas and in the developing world, where levels of health expenditure are low. The novel patented sensing technology called Android voltammetry, developed in the Hogan lab eliminates the requirement for an "instrument" and uses the existing audio capabilities of mobile phones to facilitate detection.

Our first application for this platform (the "ElecTrobe") looks set to save millions of dollars for the Australian wine industry each year. By using the audio jack to provide electrochemical stimulation we have replicated what is usually done using expensive laboratory instruments to perform "instrument free" analysis. As the data and associated metadata can be readily shared, this opens up a range of exciting possibilities for e-Health, telemedicine and "crowd sourced sensing". See http://youtu.be/X6zSgFEhFd4 and https://youtu.be/XUXvdd5nMcM. We are keen to develop new applications for this platform in the fields of environmental analysis and medical diagnostics.





Hogan group 2018 (left). Postdocs, Peter & Gina 2019 (right).

Hogan group website: https://www.latrobe.edu.au/chemistry-and-physics/research/hogan

Dr Yuning HONG

Chemical Biology

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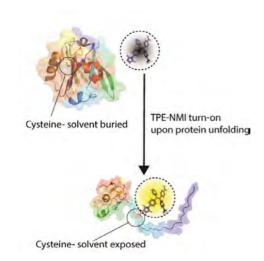
LIMS Theme: Molecular Design Positions available: Two

Fluorescence is a powerful technique that could provide spatiotemporal information with exquisite sensitivity. The primary goal of Dr Hong's research is to develop fluorescence-based tools for understanding and manipulating fundamental biological processes. Efforts will be directed towards the design and synthesis of new luminescent molecules in combination with advanced fluorescence spectroscopy and microscopy for monitoring protein misfolding and modifications associated with neurodegenerative diseases and for tracing biological events in living context.

Synthesis of orthogonal targeting chemical probes for protein labelling

Proteostasis is a housekeeping process cells undertake to maintain the proper folding and functions of proteins. Collapse of proteostasis capacity has been linked to many neurodegenerative diseases such as Huntington's, Alzheimer's and Motor Neuron

Diseases. To monitor the effectiveness of the proteostasis machinery in cells our strategy is to measure the change in the quantity of unfolded proteins of the proteome through the fluorescence output of a cysteine-reactive aggregation-induced emission probe (TPE-MI as prototype). Through mass spectrometry proteomics we can identify which proteins undergo unfolding and thus being labeled. To cover a broader proteome, this project aims to create new probes targeting lysine, tyrosine, oxidized cysteine and other post-translational modifications for profiling proteins based on their conformation and reactivity.



Relevant publications: Nat. Commun. 2017, 8, 474; CAJ 2019, 904; Angew Chem 2020, 10215.

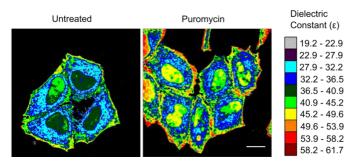
Mechanism Study of Antimicrobial Peptides by Aggregation-Induced Emission

Antimicrobial peptides (AMPs) have been considered as a rational approach to attack

target pathogens with low potential to induce *de novo* resistance in combating the emerging antimicrobial resistance (AMR). As the alternative antibacterial agents, AMPs, also known as host defense peptides (HDPs), can not only clear the invading bacteria but enhance the immune response and trigger DNA damage during infection. It highlighted the potential clinical application of AMPs with both direct antibacterial effects and indirect role of innate immunity into the therapy field of infectious diseases. It is well known that AMPs are bound to the bacterial membranes through an electrostatic attraction but the details of the AMPs membrane lytic mechanism remain elusive. Traditional fluorophores like Alexa Fluoro are usually too big in size, which could interfere with the AMP-lipid binding. They also suffer from concentration-quenching effect that hampers the application of characterising aggregation behaviour of AMPs. In this project we aim to develop small Aggregation-Induced Emission (AIE) fluorophores and label these fluorophores on AMPs to study the bactericidal mechanism of AMPs.

Self-Labeling Enzyme Tags for Measuring Microenvironment in Cells

Self-labeling enzyme tags have been an emerging technology that shows many advantages over classical fluorescent proteins for the analysis and imaging of protein-of-interest (POI). This methodology combines the specificity offered by a genetically encoded protein tag and the functional diversity afforded by synthetic chemistry. In this project we aim to combine a self-labeling enzyme tag, such as Halo-, SNAP-, CLIP-tag, with environmentally sensitive probes to study the changes in polarity and microviscosity of POI to decipher the origin of biological processes such as liquid-liquid phase separation, protein aggregation, and their interplay.



Relevant publications: Angew Chem 2020, 10215.

Techniques involved:

- Organic synthesis and characterisation
- Peptide synthesis
- Bioconjugation chemistry
- Fluorescence spectroscopy and microscopy
- Mammalian cell line culturing and transfection
- Western blotting and immunostaining
- Spectral phasor image analysis
- Mass spectrometry proteomics

Dr Adam MECHLER

Biophysical Chemistry / Nanochemistry

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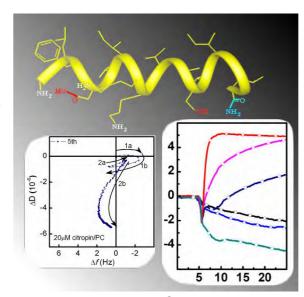
LIMS Theme: Nanoscience Positions available: One

The main research focus in the lab is using small molecule self-assembly to create nanostructures: phospholipid membranes and peptide fibres such as artificial silk. Controlling the mechanism of self-assembly through the design of the monomers and the environmental conditions is the main goal of the research. We use a range of state-of-the-art instrumentation including atomic force microscopy that can image individual molecules; quartz crystal microbalance capable of measuring the mass of a monolayer of surfactants; and microcalorimetry for measuring the phase transitions of few micrograms of material. Collaborations offer an exposure to a range of related projects.

Some of the broad research areas are outlined below.

Developing antiviral peptides

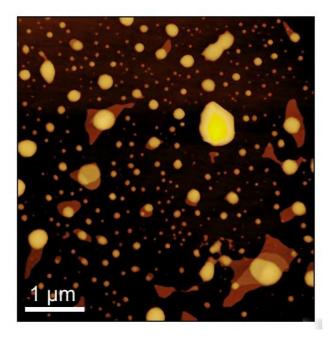
Antimicrobial peptides (AMPs) kill pathogens by disrupting their cell membranes. Several families of viruses: coronaviruses, influenza, HIV have a so called envelope, a phospholipid bilayer membrane that protects the integrity of the virus the same way as the bacterial membrane protects bacteria. Destroying this membrane "kills" the virus. Based on the data collected in the context of antibacterial activity, this project aims to repurpose AMPs to target viruses.



our group studies the mechanism of peptide-

membrane interaction, attempting rational design to improve activity. Collaborations with NUS Singapore and the Peter Doherty Institute allows us to test the activity of these peptides against actual viruses.

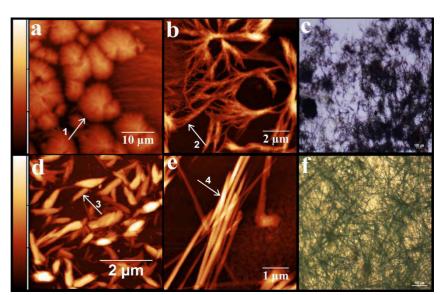
Soap bubbles and cell membranes: surfactant self-assembly



Phospholipid membranes are primarily two-dimensional self-assembled bilayer structures of surfactant molecules, held together by hydrophobic forces. We study the formation and the mechanical properties of biomimetic membranes, as well as some biosensing and biochemical applications. The figure shows an atomic force microscopy image of liposomes: filled spherical water membrane structures adsorbed to a surface. Some of the liposomes started to collapse and form flat supported membranes.

From little things big things grow: artificial silk and hierarchical nanostructures

Some peptides and small proteins assemble into fibres, such as natural silk. We are



involved in a range of projects designing and characterising selfassembling peptide based structures to create hierarchical nanoarchitectures, smart surface coatings and conductive nanomaterials. AFM imaging, quartz microbalance crystal measurements, ellipsometry, calorimetry,

fluorescence microscopy are some of the methods used in this area, with plenty of opportunities for a motivated student. The figure shows various superstructures formed by a $tri-\beta^3$ peptide.

Dr Nicholas REYNOLDS

Self-Assembling Nanomaterials

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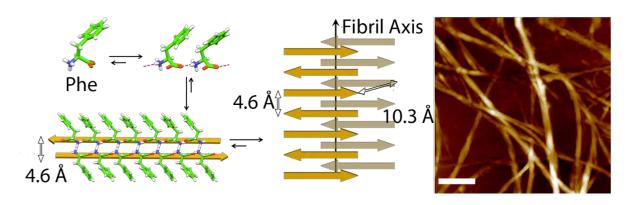
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LIMS Theme: Nanoscience Positions available: One

My lab focusses on research into the discovery and characterisation of self-assembled nanomaterials formed from various biomolecules including peptides, lipids and sugars. I use combinations of analytical techniques (Atomic Force Microscopy, Electron Microscopy, Fluorescence Spectroscopy, Synchrotron based X-ray Scattering), and molecular modelling to understand the fundamental processes underpinning the self-assembly of these materials at all relevant length scales from the molecular to the macroscale. This work has applications in understanding biomaterials design, regenerative medicine and biosensing.

Project 1: Atomic Force Microscopy Characterisation of Ultra Short Peptide Collagen Mimicking Nanomaterials



Ultra-short peptides and even single amino acids can spontaneously self-assemble into nanofibrillar structures which have applications in many technological fields including tissue engineering, biosensing and antibacterial materials. Such short peptide sequences are attractive as they are well defined, synthetically simple, and form pure nanomaterials free from contamination. In collaboration with researchers from The University of Tel Aviv we will use Atomic Force Microscopy to investigate the nanoscale morphology and

mechanical properties of a series of collagen mimicking ultra-short peptide assemblies. The nanofibrils formed by these simple peptides mimic many of the features of natural collagen and, once fully characterised and understood, are expected to have exciting applications in tissue engineering and regenerative medicine.

Project 2: Electrochemiluminescent Hydrogels for Biosensing Applications

At high concentrations the networks of nanofibrils formed from self-assembling short peptides can trap large volumes of water and form highly biocompatible self-supporting hydrogels. In this project (with the group of Assoc. Prof. Conor Hogan) we will modify self-assembled peptide hydrogels to incorporate one or more electrochemiluminescent complexes. When coated onto electrodes these luminescent hydrogels emit light in response to an applied electrochemical potential. By monitoring changes in the luminescent output of these hydrogels in the presence of various biomolecules we hope to design highly sensitive opto-electrochemical biosensors. These gels will have exciting applications in medical diagnostics, pollution detection and a range of other sensing applications.

Dr Evan ROBERTSON

Optical Spectroscopy of Atmospheric and Biological Molecules

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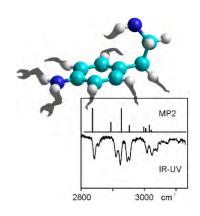
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LIMS Theme: Nanoscience Positions available: Two

Conformational shape of biomolecules

The conformational shape of biomolecules, and their interactions with the surrounding environment including water molecules, are critical to their functioning. Laser-based gas phase spectroscopy combined with ab initio calculations generates precise structural information on molecules such as neurotransmitters that provide a rigorous platform for understanding their behaviour and ultimately, rationalising drug design. The resonant two photon ionisation technique allows electronic (and IR) spectra to be measured for molecules cooled to a few Kelvin. This results in beautiful, simplified spectra that can be interpreted in terms of the possible conformers of the molecule. E.g. we discovered this neurotransmitter analogue prefers a coiled tail.

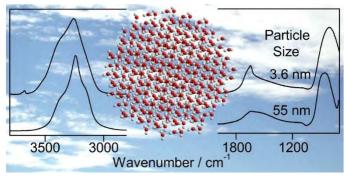




Clouds, climate, nanoparticles and spectroscopy

Aerosols play a key role in our atmosphere, affecting the climate both directly through absorption and reflection of light, and indirectly by hosting chemical reactions and influencing cloud formation. Research to investigate the formation, composition and behaviour of aerosols is critical to improve the climate models. Infrared spectroscopy is important because it is widely used to monitor chemical species found in the atmosphere, and because interactions with IR radiation are crucial to earth's energy balance. A specialised cooling cell with unique capabilities at the Australian

synchrotron's IR beamline has enabled us to measure the first far IR spectra of water ice nanoparticles. Such particles as are found in cirrus and mesospheric clouds on earth, and in non-terrestrial environments such as Mars, Titan and the interstellar medium. We are now exploring the effect of trace acids on the spectra of icy nanoparticles



Raman Spectroscopy

Raman spectroscopy has become a widely used technique for chemical analysis and molecular characterisation. It measures vibrational levels in samples and is a complementary to IR spectroscopy. In the LIMS laser lab we have a Raman microscope that is one of the few in Australia equipped with a UV laser source.

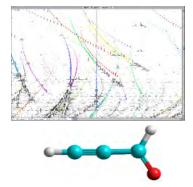
Recent interest has included not only characterisation of traditional chemical samples but projects based on structural insights into peptides, examination of oxalates in leaves, melanin in spiders and iron minerals in archaeological samples.

Millimetrewave and high resolution synchrotron IR spectroscopy

The synchrotron IR work is conducted to obtain rovibrational properties of gaseous atmospheric molecules (allowing their IR absorption profiles to be modelled), and interstellar molecules.

Over 100 molecules have been detected in space, mostly from their rotational spectrum measured by radiotelescopes. Instruments operating in the millimetrewave region are now revealing thousands of unidentified lines. Some of these mystery lines will be from as yet unidentified molecules but others are "weeds". These are from known interstellar species but derived from isotopolgues or "vibrational satellites" that have not yet been characterised in the lab. One project would be to assign and analyse transitions of propynal, and hence contribute to the identification of unknown interstellar spectral lines.







Dr Pallavi Sharma

Synthetic Organic Chemistry

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LIMS Theme: Molecular Design Positions available: One

Sharma Group expertise in the development of new chemical methodologies to access novel chemical scaffolds with function. We champion the use of under explored reagents for the construction of rare and complex molecular scaffolds under environmentally benign conditions.

For more information see: Org Lett. 2018, 20, 4263. Org. Lett., 2016, 18, 1100.

Leaving Flat Land: Synthesis and application of 3D-Scaffolds

Novel chemical entities with function are fundamental to medicinal, biological, material and agricultural sciences; hence they are essential to sustain the healthcare sector, meet energy demands and maintain food security on a global scale. Rigid, 3-dimensional molecular scaffolds, which provide unique entry to under-explored regions of three-dimensional chemical space, have recently formed an indispensable tool in the search for new lead compounds, with spirocyclic compounds occupying a prominent position in this area. Current research in Sharmalab is built upon our foundation work on the utilisation of cyanamide reagents for the construction of rare heterocycles. We further aim to expand these rare heteroatom rich cyclic systems into structurally complex and unprecedented 3D-spiro-heterocyclic rings. Making use of highly efficient and robust 'click-type' dipolar cycloaddition chemistry, a host of new structures will be synthesised targeting application in the field of drug discovery, biological and material science, sensor and catalysis.

Application: Drug Discovery, Material Science, Sensors, Catalysis.

Techniques used: Organic Synthesis, Dipolar Cycloaddition, Fluorescence spectroscopy, Enantioselective Synthesis, HPLC, React-IR and Method Development.

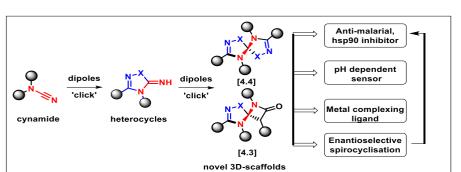


Figure1:
Synthesis and application of novel 3D-scaffolds

Professor Brian SMITH

Modelling Molecular Interactions

Professor, Dean and Head of the School of Molecular Sciences

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LIMS Theme: Molecular Design Positions available: One Hons/MSc

Molecular modeling plays an integral role in the discovery and development of new drugs, being a key component in the process of structure-based drug design, in aiding in the identification of molecules in lead discovery and in predicting pharmacokinetic properties. We utilise quantum-mechanical methods to understand enzyme mechanism; molecular mechanical methods to explore the dynamics of proteins; and use a variety of tools to predict how molecules interact. We employ X-ray crystallography to determine the structures of complexes of proteins, polypeptides, and small molecules.

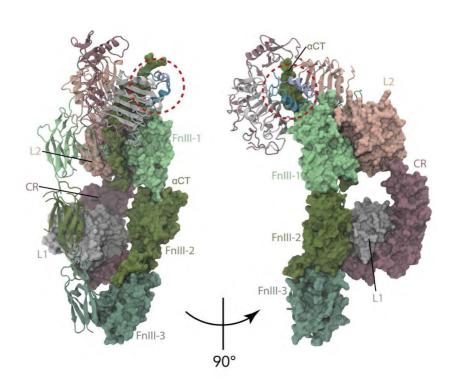
Laws of attraction and repulsion: a novel family of bacterial chemosensors.



Chemotaxis plays an important role in the ecology of bacterial populations. The aim of this work is to determine the mechanism of how a newly characterised, widespread family of chemotaxis receptors sense and discriminate between attractants and repellents, and transduce the signal across the membrane. It is anticipated that this knowledge will drive the discovery of new chemoeffectors and the redesign of receptor specificity, with the aim to control movement of bacteria for numerous applications; e.g. to direct biodegrading bacteria towards sites of contamination, repel pathogenic bacteria from the endangered coral reef, enhance symbiotic association of nitrogen-fixing bacteria, or prevent bacterial build-up on implanted medical devices.

Engineering novel insulin mimetics

Although the three-dimensional structure of insulin has been determined since the 1960's, and the structure of the hormone in complex with the insulin receptor (IR) having been determined in 2018, much is still unknown about the structural and functional relationship of the peptide and its interaction. An integral homoeostatic hormone, and a life-saving therapeutic given to patients suffering from diabetes mellitus, significant detailed computational investigations on the peptide and its interaction are limited, in no small part the result of the absence of structural details. Understanding how insulin changes conformation to bind the IR, and further exploitation of this interaction, are both key in designing new insulin-based therapeutics. The recent exploitation and investigation of both long acting and stable single-chain insulin analogues, and of short fast-acting cone snail derived insulins are two examples of this. This project will focus on investigating the insulin peptide, using high performance computing to simulate the features which facilitates is high efficacy at the IR.



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Computational Chemistry

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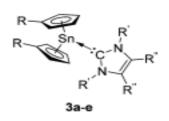


LIMS Theme: Molecular Design Positions available: Two

Our group "does chemistry by computer" to understand the structures and properties of molecules and how they react. We focus on the chemistry of important molecules, molecules with unusual bonding environments, and the prediction of new and novel chemistry. The projects listed here are examples of available projects.

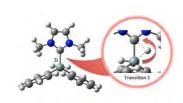
(1) Predicting new chemistry and probing novel bonding environments. Carbenes are one of the most important new class of molecules discovered in the last decade. The field of main group carbene chemistry is exciting with new discoveries constantly being made. Together with Dr Dutton we have proposed a series of main-group molecules that are inherently unstable but can be stabilised by ligands (e.g. L-EE-L; E = main group element, L = carbene ligand). These molecules have a donor-acceptor bonding form (like metal coordination complex). There are current projects focused on i) beryllium chemistry (see artwork to the which is chemically poisonous but is perfectly safe on a computer; (ii) designing new and novel carbene ligands; (iii) using carbenes to propose new bonding such as B-C triple





bonds; (iv) metal compounds with donor ligands, including carbon acting as a bidentate ligand.

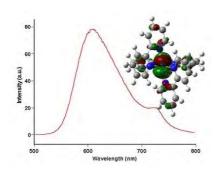
(2) Modelling reaction mechanisms to understand reactivity. There are a number of projects in this area, such as (i) reactions of borole rings with unsaturated molecules (*Inorg. Chem.*, 54, 8957, 2015), (ii) insertion of carbenes into Si-H bonds of R-SiHCl₂ (*Inorg. Chem.*, 55, 1953, 2016), or (iii) nickel-catalysed



borylation of fluoro-aryl groups by C-F bond cleavage (JACS, 138, 2016, 5250).

(3) Metal-containing systems that absorb/emit light.

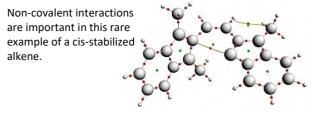
(i) The development of light-emitting diodes (LEDs) and sensors is a hot topic of chemical research, for which metal-based (eg. iridium, ruthenium) materials are ideal targets. These are purely computational projects in collaboration with experimentalists including Prof Paul Francis (Deakin), A/Prof Conor Hogan and Dr Barnard. We model



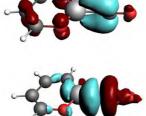
luminescence and can model phosphorescent lifetimes, in addition to UV-Vis spectra, MO and redox properties. (ii) Gold chemistry: we are interested in understanding aurophilic (Au-Au) interactions, which are responsible for some of the fascinating properties of gold. (iii) A triple-decker ferrocene sandwich compound has recently been reported, for which we will investigate its properties.

- (4) High-accuracy energetics and properties. These projects are focused on accurate energies and properties where we can push the limits of computational chemistry methods, which has relevance to different areas of chemistry. We can produce results as good as, sometimes better than experiment! Our goal is for reaction energetics to an accuracy of 1 kJ/mol, and NMR shifts to better than 1 ppm. Projects include (i) NMR shielding including ¹⁹F, ⁹Be, and ¹⁵N; (ii) correct the inaccurate experimental energetics of imines reported by Peerboom (*Perkin Trans.* 2, 1825, 1990); (iii) investigate the requirements for the accurate calculation of redox and acid/base properties of luminescent materials; (iv) development and/or testing of new basis sets; and (v) assessing the anharmonicity of N-F bonds and its impact on molecular properties.
- (5) Modelling organic and biomolecules in the gas phase. We model gas-phase molecular properties of biologically important molecules (e.g. amino acids), which links high-level computational methods with new experimental techniques (e.g. collaboration with Dr Robertson). Our group has significant experience in modelling natural and modified amino acids in the gas-phase. One potential project is to investigate the properties of amino acids whereby the N is replaced by P atoms.

All students will develop an advanced understanding of chemical structure and reactivity, develop enhanced analysis and problem-solving skills, and have the likelihood of publication of your research in an international chemistry journal.



We can plot individual orbital interactions to understanding bonding: electron density flows from red to blue, with π back-bonding (top) and σ donation (bottom).



PHYSICS PROJECTS

Professor Brian Abbey

Coherent X-ray Science and Materials

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Dr Connie Darmanin

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LIMS Theme: Nanoscience Positions available: Two

Our research is focused on the development of novel approaches to imaging and characterising materials and biological structures at the atomic, molecular and cellular level. In our research we utilise the latest developments in imaging technologies aimed at delivering information from molecular systems on a femtosecond timescale. Our goal is to enable Australia to be an international leader in X-ray imaging, to train next generation interdisciplinary scientists and to provide new insights for combating common diseases that afflict society. Activities within our group are focused around the following areas:

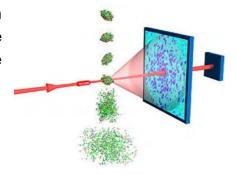
Synchrotron and X-ray Free Electron Laser Science (XFEL)

X-ray crystallography is routinely used to determine protein structures. However, serial crystallography at synchrotron and XFEL sources are creating new opportunities in this area by enabling structure determination from microcrystals and nanocrystals. Structure determination via serial crystallography is achieved by injecting randomly orientated crystals into a reaction zone traversed by the X-ray beam (shown in figure). Orientations may be classified by examining Bragg spots and assembling them into a three-dimensional diffraction volume.

We have a number of projects available in the area of synchrotron and XFEL science.

Research within our group involves both the development of new approaches to data collection and advancing serial crystallography methods for delivering crystals into the X-ray beam. Please contact Dr Connie Darmanin (<u>C.Darmanin@latrobe.edu.au</u>) if you are interested in becoming involved in this research.

<u>Outcomes</u>: This work will permit structure retrieval from the smallest possible nanocrystals and provide opportunities to be involved in serial crystallography at the Australian synchrotron and international facilities.



Optics and Nanofabrication

Characterisation of biomolecules as they undergo diffraction, the development of next-generation X-ray optics, and the delivery of single cells and molecules in single-particle imaging experiments all require state-of-the-art nanofabrication techniques. Our group uses a range of techniques including optical ptychography, focused ion beam (FIB), atomic force microscopy (AFM) and chemical vapour deposition (CVD) as part of its optics and nanofabrication program. We have a number of projects aimed at developing devices that can characterise tissues and single molecules and for the characterisation and injection of single particles into X-ray beams.

<u>Outcomes</u>: The development of new methods for characterizing tissues as well as visualising single molecules and their dynamics.

Dr Narelle Brack

Nano-structure Materials, Interfaces and Surface Science

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Theme: Nanoscience Positions available: One

The research activities of this group focus on creating, understanding and controlling materials at the nanometer scale. We have a strong focus on surface science exploring chemical and molecular properties and processes at surfaces and at interfaces. Surface modification strategies have been designed and developed for a diverse range of material systems including next generation aircraft materials and carbon nanomaterials.

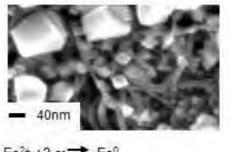
Iron-Carbon Nanomaterials: the influence of nanoscale interactions on magnetic properties

This project focusses on the deposition and growth mechanisms of Fe layers on technologically relevant carbon nanomaterials in order to develop reliable, controllable and industrially scalable production methods for magnetic nanomaterials. The primary focus areas of the research project are

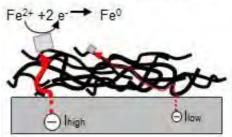
- Surface functionalisation of carbon nanomaterial
- Design of novel electrodynamic deposition methods
- Nanoscale structural and surface chemical characterisation, and
- Correlation of the chemical, structural and magnetic properties

New magnetic nanomaterials will be designed and characterised at the molecular level. This study targets the major scientific challenges of practical and scalable processing techniques for nanomaterials and establishes experimental designs based on controlling chemical, interfacial, structural and magnetic interactions. The Honours project will focus on selected aspects of this larger project.

The research program involves researchers from four key organisations, La Trobe University, RMIT University, Defence Science and Technology Group (DSTG) and The Australian Synchrotron.

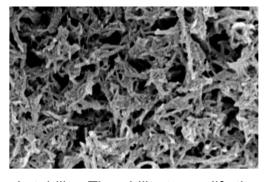


Please refer to our publication: Brack N, Kappen P, Herries A I R, Trueman A and Rider A N 2014 Evolution of magnetic and structural properties during iron plating of carbon nanotubes *J. Phys. Chem.* C **118** 13218-27



Thin Film Deposition of BNNTs for Sensing Device Applications

Boron nitride nanotubes (BNNTs) have been increasingly investigated for use in a wide range of applications due to their unique physicochemical properties including high hydrophobicity, heat and electrical insulation, resistance to oxidation and hydrogen storage capacity. They are close structural analogues of carbon nanotubes, however, they possess a much wider band gap (~5.5 eV), exhibit



higher resistance to oxidation and show greater thermal stability. The ability to modify the band gap by an external electric field make BNNTs an attractive candidate for electric-optical (EO) modulation sensing device applications.

The initial goal of the current study is to develop methods for thin film deposition of BNNTs that are adaptable to the preparation of sensor devices. Processes that can provide uniform and controlled thickness films are required to produce reliable sensor devices. Electrophoretic deposition (EPD) is an ideal technique to trial for thin film production due to its reliable, precise and scalable characteristics. Initial studies will examine different functionalisation techniques for the boron nitride nanotubes to create stable aqueous dispersions which are suitable for EPD. After successful EPD methods have been developed, post-deposition doping will be used to adjust the bandgap of the films. XPS and SEM will be used to characterise the chemistry and morphology of the films.

Dr David HOXLEY

Low-dimensional Electronics and Biosensing

Senior Lecturer

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Theme: Nanoscience **Positions available:** None in 2021

Towards implantable diamond biosensors

The field of implantable biosensors is progressing at a cracking pace, for good reasons. Continuously monitoring the bodies of patients allows them to receive the best possible treatments. Doing so outside the hospital environment offers the best quality of life (and significantly reduces treatment costs). These projects explore a big challenge: how to functionalise a biocompatible surface so that it is selective, sensitive, stable and long-lived. Diamond is highly stable and biocompatible but as an emerging electronic material, much remains to be known about crafting working devices.

Mesoscale electronic circuits in diamond

The diamond surface can be made conductive by adsorbing hydrogen. The student will use an Atomic Force Microscope to 'draw' electrical pathways and devices in areas less than the width of a hair.

Laser-induced conductivity of functionalised diamond surfaces

An implantable biosensor should have no wires breaking the skin. But how then to get power in and information out? The student will investigate how pulsed lasers can be used to interface with the biosensor through the skin.

NEXAFS of ECL compounds

Electro-Chemi-Luminescent compounds show exceptional charge transfer properties within their molecules. NEXAFS is a synchrotron-based technique which can reveal whether charge transfer occurs to the diamond surface, thus functionalising it. The student will analyse existing synchrotron data, and will also work with beamline scientists from the Australian Synchrotron.

Electrical properties of nanostructured surfaces

Photovoltaics have moved well beyond silicon solar cells, promising ever greater harvesting of energy from our nearest fusion reactor, the sun. Both organic and inorganic approaches require careful understanding of the nanoscale electrical properties of the films at the interface layers. The Atomic Force Microscope in electrical characterisation modes can be used for this, and combined with macroscopic techniques to relate the effects at different length scales.

Electrical properties of LiF at high temperatures

LiF is an extreme material, and is an important component of photovoltaics and power storage devices. Strange things happen at high temperatures.....

Conductivity of Ag Nanowires

Silver is a popular material amongst nanotechnologists, and ultra-narrow wires can be grown with minimal effort. The properties of these wires is of great interest, particularly when heated. This project will be done in collaboration with Daniel Langley.

Electrical characterisation of ZnO nanostructures

Many advanced inorganic photovoltaics rely on an ultrathin zinc oxide structures to get charge out of the device. These structures need to conduct electricity in just the right way. The student will characterise a range of ZnO nanostructures grown by collaborators to give feedback into optimising growth recipes.

Electrochemistry of Pyrite under fluids

Pyrite is an abundant natural semiconductor with, theoretically, very good photovoltaic properties. In practice, defects and surface effects are a barrier to working devices. This project will attempt to work out what these effects are, and how to get around them. Along the way, it may shed some light on how to combat acid mine drainage, a very significant environmental problem.

Dr Shanshan Kou

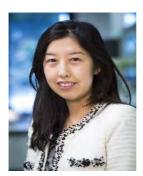
Biophotonics

Lecturer

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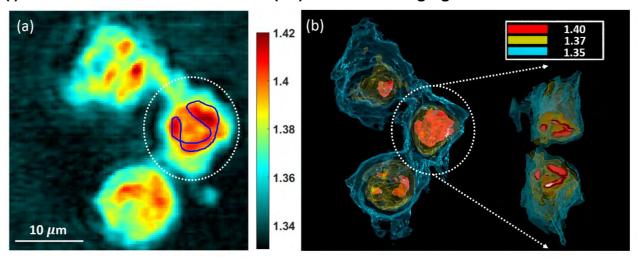
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Theme: Nanoscience Positions available: Two

My research is focused on the highly interdisciplinary domain of bio-photonics and bio-imaging using optical microscopy and nanotechnology. We use light to probe cellular and molecular samples to obtain quantitative photonic signatures such as phase, refractive index, wavelength, phase, polarisation etc. The goal is to investigate these biophysical properties and relate them to the cellular, sub-cellular and molecular mechanisms and pathways, which will in turn offer insights into biological case studies and biomedical diagnostics.

(I) Label-free Three-Dimensional (3D) Structural Imaging in Cells

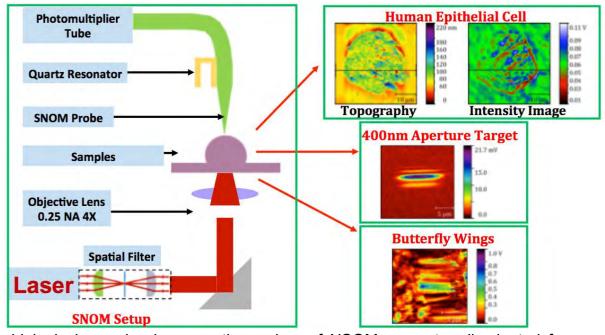


Label-free 3D imaging through tomography shows cellular structural information from intrinsic contrast mechanism. Such dynamic structural and morphological information may give rise to previously unavailable biomedical data that can improve our understanding of the complex cellular mechanisms in some critical aspects of cell studies, such as their death and degeneration, metabolic activity, or drug reaction. We have successfully demonstrated its application in observing morphological changes in cell

death. A honours position is offered to have a first-hand experience with this advanced microscope and look into a real case study for cells.

(II) Near-field Scanning Microscope for Cellular Studies

The near-field scanning microscopy (NSOM) is a versatile tool to achieve nanometric scale resolution. To date, however, little is studied for its capacity with cellular and



biological samples because the probes of NSOM are not well adapted for aqueous environment. In collaboration with a team of experts in RMIT University, we are devising custom-made probes for the NSOM and will be pioneering the research into NSOM for cellular studies. A honours position is offered to participate in this exciting project with a focus on the experimental skills.

Outcomes: The applicants are expected to receive training and make impactful research in various hot topics of biophotonics, and participate in a highly interdisciplinary research environment that involves biomedical instrumentation, computer modeling, nanotechnology, biological science and photonics.

Professor Chris Pakes

Diamond Research Group

Professor

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Dr Alex Schenk

Diamond Research Group

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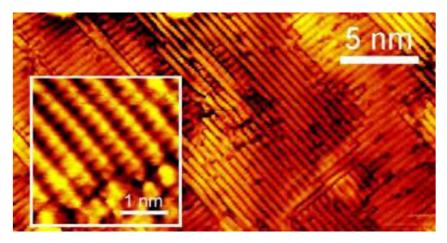
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Theme: Nanoscience Positions available: Two

Research in our group focuses on developing diamond as an electronic material. We tune the electronic structure of the diamond surface via chemical modification and surface transfer doping in order to induce desired electronic properties. Diamond devices are engineered for the study of phase coherent quantum transport including spin transport and superconductivity, for applications in sensing, low-power electronics and quantum information.

Our experimental studies utilise a variety of complementary techniques. Surface modification and characterisation studies are performed using a combination of ultra-high vacuum scanning probe microscopy and synchrotron-based photoemission at the Australian Synchrotron. Our laboratory houses two ultra-high vacuum scanning probe instruments, permitting atom-scale imaging, manipulation and spectroscopy at temperatures down to 10 K. These systems are additionally equipped with instrumentation for molecular dosing, four-point probe conductivity measurements and Low Energy Electron Diffraction. We are regular users of the soft X-ray spectroscopy (SXR) beamline at the Australian Synchrotron, where we use the high-resolution and surface sensitivity offered by this facility to characterise the electronic properties induced by our chemical functionalisations, and the electronic properties of molecular dopants on the surface.



Rows of carbon dimers on the hydrogen-terminated (100) surface of diamond

Current activities in this area include, but are not limited to, the development of siliconterminated (100) and (111) diamond surfaces, which possess new electronic and structural properties. Additionally, we are working extending towards our STM imaging capabilities with unconventional imaging modes such as resonant electron injection, and seek to use STM to controllably remove individual hydrogen atoms from the hydrogenterminated (100) diamond surface, in a manner similar to that already demonstrated on hydrogen-terminated silicon, allowing for atomically precise manipulation of the surface electronic structure atom-scale and engineering of molecular surface devices.



Createc low-temperature scanning tunneling microscope

Surface functionalisation provides a route to developing interesting electronic properties and we are particularly interested in the two-dimensional electronic systems that exist at the surface of hydrogen-terminated diamond and may exist at the surface of silicon-terminated diamond. To explore the quantum transport behaviour of these systems we fabricate Hall-bar and gated (FET) devices and explore their electronic behaviour in high magnetic fields and at very low temperatures (to 50 mK). In this area, we have recently shown that hydrogen-terminated diamond supports a two-dimensional *p*-type surface conductivity that possesses a high spin-orbit interaction. With its unique spin properties, this finding is of significant interest to the spintronics community.



We are developing this project through a number of avenues that seek to demonstrate device architectures that permit tuning of the spin-orbit interaction, possess high charge carrier mobility, and exhibit superconductivity at low temperature.

Our group hosts several PhD researchers who often work collaboratively on different aspects of the same project and material.

Professor Paul Pigram

Complex Materials, Interfaces and Surface Science

Professor; Director, Centre for Materials & Surface Science

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Theme: Nanoscience Positions available: Two plus

The research activities of this group focus on creating, understanding and controlling complex materials at the nanometer scale. We have a strong focus on surface science, in particular exploring chemical and molecular properties and processes at surfaces and at interfaces.

We have multiple project opportunities available in the field of surface science, surface analysis and precision materials fabrication including projects involving deep collaboration with CSIRO Manufacturing and embedded student activities with key industry partners.

Projects access the state-of-art surface analysis instrumentation of the *Centre for Materials and Surface Science (CMSS)* at La Trobe

https://www.latrobe.edu.au/surface/

Examples of project opportunities include:

Plasma polymer based metal affinity coatings for ELISA (in collaboration with CSIRO Manufacturing)

Immobilised metal affinity chromatography (IMAC) is a biochemical based separation technique commonly employed in protein separation. Translation of IMAC into microarray and microfluidic technology would see significant improvements in processing times, reagent volumes and overall efficiency. CSIRO researchers have previously shown that plasma polymers can be used to bind metal ions and subsequently bind functional biological proteins selectively.

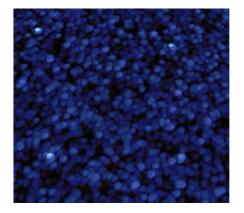
We are investigating the fundamental mechanisms of metal and protein binding to the plasma polymer surfaces and optimising the surface, metal, metal-ligand and protein chemistries to achieve optimal performance of the surface bound proteins in enzyme linked immunosorbent assay (ELISA) screening and protein ligand-cell based screening assays. This research, based on the principles of IMAC, Immobilised metal affinity chromatography, is investigating the fundamental mechanisms of metal and protein

binding (via XPS, ToF-SIMS and the use of recombinant proteins, supported by extensive multivariate analysis including machine learning and artificial neural networks) to the plasma polymer surfaces and optimise the surface, metal, metal-ligand and protein chemistries to achieve optimal performance of the surface bound proteins in enzyme linked immunosorbent assay (ELISA) screening.

Predicting positive responses to cancer treatment with machine learning (in collaboration with Olivia Newton-John Cancer Research Institute)

The group has a very successful multidisciplinary project in progress with Dr Suzi Cutts (La Trobe Biochemistry) and the Olivia Newton-John Cancer Research Institute (ONJCRI). Anthracyclines such as doxorubicin are among the most effective chemotherapy agents for the treatment of a wide variety of cancer types. Although many mechanisms of action have been proposed, it is broadly accepted that the primary mechanism of action in cancer cells involves DNA damage. However, doxorubicin also attaches covalently to DNA in a reaction that is mediated by formaldehyde.

The group has demonstrated that the delivery of formaldehyde via suitably designed pro-drugs greatly enhances the rate of cell death. This raises the possibility that efficient and specific delivery of pro-drug to cancer cells, for example using a nanoparticle delivery system, might allow lower doses of doxorubicin to be administered. This in turn has the potential reduce the incidence of cardiotoxicity associated with doxorubicin use and extend patients' lives.



The systems are being characterised using molecular and biomolecular imaging and analytical approaches including confocal microscopy, ToF-SIMS, XPS and AFM. These studies will be supported by multivariate analysis including principal components analysis, cluster analysis and self organising maps.

Next generation concrete technologies: engineering solutions, asset management and sustainability (in collaboration with the SmartCrete CRC)

The newly launched SmartCrete CRC will launch a new generation of technologies for Australian industries making, using and relying on concrete. A range of project opportunities are available considering materials composition and behaviour, sensing, corrosion, through-life performance, large scale data science and materials recycling, upcycling and reuse.

Dr Chanh TRAN

X-ray Physics

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Theme: Nanoscience Positions available: Two

Our research is in the fields of X-ray Optics and Interactions of X-rays with Matter: Synchrotron Science, Coherence Studies, X-ray Imaging and Interferometry, Precision Measurements of Interaction Cross-sections of X-rays with Matter. The projects will generally require a combination of experimental and analytical skills.

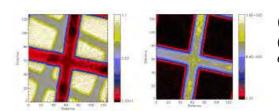
X-Ray Coherence and Imaging

This project aims to develop techniques for extracting the maximum possible information conveyed in optical fields. Partially incoherent fields contain far greater information capacity compared to fully coherent fields (e.g. lasers). A fundamental limitation of current imaging techniques is the lack of a technique that is capable of extracting the enormous amount of information carried in partially optical wavefields. The research program will apply techniques such as Phase Space Tomography [Opt. Lett. **30** 204-206 (2005); JOSA A **22** 1691 (2005); Phys. Rev. Lett. **98**, 224801 (2007)] to develop state-of-the-art X-ray imaging technique in which all the information about an object encoded in a partially incoherent wavefield can be decoded or reconstructed. The project is fundamentally important and also promises great potential applications.

Complete reconstruction of the phase-space function of an X-ray wavefield defined by a 1D single slit.

Elemental Contrast Full-Field Imaging

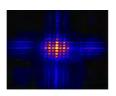
In many frontier areas of research it is the distribution of a particular element in the sample which is of crucial interest. This project aims to develop the elemental contrast full-field imaging method recently proposed [Phys. Rev. A **78** 13839 (2008)]. Rather than comparing the images measured above and below an absorption edge in conventional absorption contrast technique this method enhances the phase effect due to a particular element by taking multiple-wavelength measurements in the vicinity of its absorption edge. The method can be incorporated to various techniques of X-ray full-field imaging and therefore promises a wide range of applications.



(Left) An intensity image of a 2 component sample.
(Right) Reconstruction of the projected thickness of a single element of the compound sample using this technique.

X-ray interferometry

Various forms of interferometry-based techniques can probe both amplitude and phase changes in wavefields in a very sensitive, precise and powerful manner. This project aims to develop 'non-destructive' interferometric imaging techniques for quantitative studies of phase systems with significant improvement in sensitivity and precision.



Two-dimensional interference intensity distribution of an x-ray beam defined by four square pinholes. Profiles and positions of the interference peaks are very sensitive to, and can be used to reconstruct the complex refractive index profile of an object inserted in one of the pinholes.

Elemental Contrast Tomography

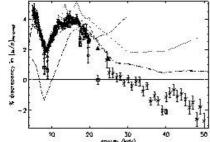
This project aims to explore the application of Elemental Contrast Full-Field Imaging to X-ray tomography. The development of this combined technique provides a unique tool to achieve 3D elemental contrast of compound samples and therefore promises great uses in many important research areas including manufacturing, material sciences, mining industry and cellulous studies. The project requires a combination of experimental, computational and analytical skills.

Interaction of X-rays with Matter (photo-absorption, scattering, fluorescence)

This project involves critical study of atom-photon interactions by accurate determination of the complex atomic form factors. Photon-atom interaction cross-sections are important in many fields of fundamental and applied physics. As many uncritical applications are well established, researchers and users outside the field have assumed that experiment and theory have converged with no further critical goals in this area. This assumption is seriously flawed for all elements in many energy regions.

Discrepancies in the total attenuation coefficient of silicon between our work using the XERT (solid circles), other experiments (symbols) and theories (lines). The significance of the results was discussed in Phys. Rev. Letts., 90, 257401 (2003).

We have developed a novel experimental technique called the X-ray Extended Range Technique (XERT) for



accurately determining these cross-sections. The project will apply XERT in the investigation of the angular dependence of X-ray scattering, which probes wavefunction distributions, bonding, shake-up and shake-down processes and which is at the forefront of modern atomic physics. The project requires a solid theoretical background and good experimental skills.

Dr Grant van RIESSEN

X-ray Microscopy and Condensed Matter

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Theme: Nanoscience Positions available: Three

Research in our group is focused on creating new ways to characterise and manipulate materials at the nanoscale using coherence synchrotron light sources. We develop new instruments, experimental techniques and algorithms that enable advanced lithography, imaging and metrology. We apply the imaging methods to study in situ physicochemical dynamics of nanostructured functional materials. We lead the development of extreme ultraviolet nanolithography facility that will produce the smallest structures every produced by light.

Opportunities for Honours and Masters students are available in project areas detailed below. A student joining our group can expect to become proficient in laboratory techniques and modern approaches to numerical modelling and data analysis that are commonly required in experimental physics research. Most projects will offer students the opportunity undertake part of their research at synchrotron radiation facilities and external nanofabrication laboratories.

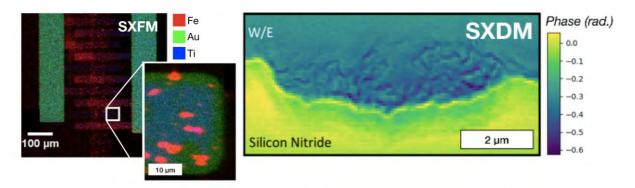




The soft X-ray imaging facility operated by our group at the Australian Synchrotron (left) and students preparing samples at the Melbourne Centre for Nanofabrication cleanroom.

In situ X-ray microscopy of electrochemical processes

We have developed fast nanoscale imaging techniques based on the combination of scanning X-ray diffraction microscopy (SXDM), scanning X-ray fluorescence microscopy (SXFM) and X-ray absorption spectroscopy. These are applied to in situ characterisation of the morphological structure and chemical composition of materials relevant to energy storage technologies. Current developments are focused on optimising SXDM using recently available detector technology capable of recording high dynamic-range diffraction data at kHz frame rates in the hard X-ray regime. Massively parallel image reconstruction algorithms that take advantage of data redundancy across multiple dimensions are being developed for real-time imaging of dynamic processes with low X-ray dose and high sensitivity.



The distribution of Fe electrochemically deposited on Au electrodes of microfabricated, thin-film electrochemical cell (left). SXDM images of similar electrodes (in solution) show nanoscale morphology of Fe-CNT composites formed during electrodeposition.

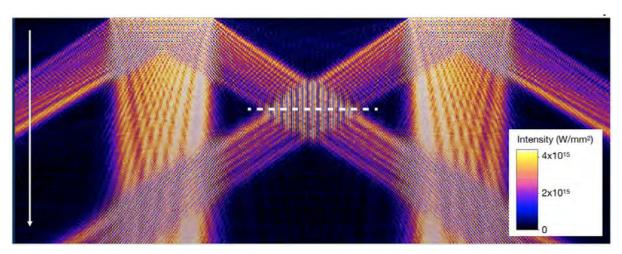
Development of EUV interference lithography gratings

High-resolution (<20 nm) gratings with high diffraction efficiency, geometric uniformity and very low defect density are required to achieve our goal of producing single-digit nanometer resolution with EUV interference lithography (IL) using a facility being developed in collaboration with ANSTO, CSIRO and other Universities. EUV-IL using 13.5 nm illumination currently faces a number of challenges associated with the grating mask technology, including poor diffraction efficiency and critical dimension distortions that result from surface and interface roughness. These issues are more critical at shorter wavelengths required for the next generation of EUV lithography.

New processes for fabricating grating masks suitable for EUV-IL over the wavelength range 6.7—13.5 nm are currently being developed in partnership with the MCN. Project opportunities exist for students who able to regularly undertake work with a co-supervisor at MCN, focusing on optimisation of either $Mo_{1-x}N_x$ thin-film absorber patterning by electron beam lithography, or the preparation of ultrathin Si and BN membranes.

Simulation and modelling of extreme ultraviolet lithography with partially coherent synchrotron radiation

Comprehensive modelling of the of the imaging branch of the Soft X-ray Spectroscopy beamline at the Australian Synchrotron is required to support the development and optimisation of extreme ultraviolet interference lithography (EUV-IL) and in situ metrology capabilities. Using high-performance computing it is possible to numerically propagate a partially coherent wavefront from a model undulator light source, through beam transport optics and model photomasks. Analysis of the simulated irradiance of the wavefield at the plane of the photoresist (the aerial image) provides insight into role of partial coherence, polychromaticity, and polarisation. At the current stage of this project we are using this numerical modeling approach to inform the material choices, geometric design and defect tolerance of multilayer photomasks for short wavelengths (6.7 nm). Models developed will also be used to support the analysis of data obtained during the experimental evaluation of the optical system and photomask prototypes.



Simulation of image formation in EUV interference lithography. A coherent EUV wavefront from a model undulator light source is numerically propagated through a grating mask to study how the periodic interference pattern that forms where diffracted beams interfere (dashed-line) may be transferred to photosensitive films.

CHEMISTRY/PHYSICS/NANOTECH PROJECT SELECTION FORM



lame:		Student Number:
Phone:	Email:	

You must consult a minimum of **three (preferably four)** research advisors and obtain their signature before submitting your form. Please number your preferences starting from 1.

	Research Group	Signature of Supervisor	Preference
Chemistry	Research Skills Project		
	B. Abbott		
	C. Abrahams		
	P. Barnard		
	J. Dutton		
	C. Hogan		
	Y. Hong		
	A. Mechler		
	N. Reynolds		
	E. Robertson		
	P. Sharma		
	B. Smith		
	D. Wilson		
Physics	B. Abbey		
	N. Bracks		
	D. Hoxley		
	S. Kou		
	C. Pakes		
	P. Pigram		
	C. Tran		
	G. van Riessen		

Please return the completed form to an Honours/Masters coordinator (Pallavi Sharma, Peter Barnard, Grant van Riessen) or the School of Molecular Sciences Administration Office (Room 201, LIMS1) via email by

Friday 6th November 2020

Please note that the academic signature indicates that you have discussed projects with the academic rather than a commitment to supervise you. Allocations of supervisors are made on the basis of supervisor availability, student preferences and student marks.

General enquiries

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