THE UNIVERSITY OF MELBOURNE

School of Chemistry

Faculty of Science

Chemistry Research Prospectus

Contents

About the School

The School of Chemistry is dedicated to improving our world and training outstanding graduates in chemistry.

We research functional materials, chemical biology, sustainability and the environment with cutting-edge knowledge and technology.

Advanced knowledge in chemistry is essential for building a sustainable future. We address major societal challenges in energy, environment and health through education, research, training, and engagement.

The University of Melbourne's Faculty of Science acknowledges the Traditional Owners of the lands on which we work: the Wurundjeri Woi-Wurrung and Bunurong peoples (Burnley, Fishermans Bend, Parkville, Southbank and Werribee campuses), the Yorta Yorta Nation (Dookie and Shepparton campuses), and the Dja Dja Wurrung people (Creswick campus). We pay respect to their Elders, past and present. We also acknowledge and respect that Aboriginal and Torres Strait Islander people are this country's first scientists, with deep and enduring knowledge of the land, waters and skies.

Professor Muthupandian Ashokkumar

Head of the School of Chemistry

Professor Muthupandian Ashokkumar

- Ultrasonic technology
- Food and bioprocessing
- Biofunctional materials

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My fundamental and applied research work involves multi-disciplinary areas involving ultrasonic technology, materials chemistry, surface chemistry, photochemistry and spectroscopy. My focus has been to address energy, environment and health.

Using my expertise, I intend to develop ultrasound-based technologies for: 1. Synthesising nanomaterials for energy production and biofunctional materials for improving human health and wellbeing, and 2. Bioprocess industries to manufacture marketable food and health products.

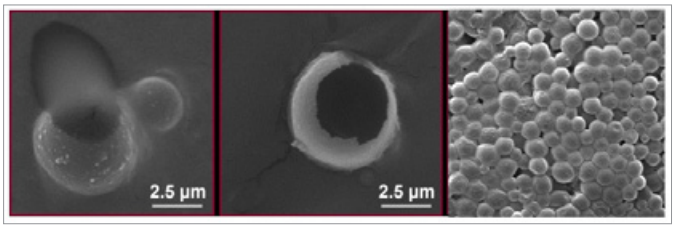
Ultrasound-assisted fabrication of biofunctional materials

Biofunctional core-shell materials (microspheres) are widely used for the encapsulation and targeted delivery of drugs in diagnostic and therapeutic medicine. They can also be used for the encapsulation and efficient delivery of value-added food ingredients, such as flavours and nutraceuticals. My research focuses on the sonochemical synthesis of biofunctional core-shell materials for the encapsulation and delivery of biofunctional compounds, such as vitamins, food flavours and aromas. We recently completed a proof of concept study (funded by a Bill & Melinda Gates Foundation Grand Challenges Explorations Phase I Grant) involving the encapsulation of nutrients inside edible microspheres using ultrasonic technology. This project addressed the issue of infant and maternal malnutrition in developing countries by reducing the cost of staple food fortification using novel edible nutrients-loaded microspheres. A second target application that we are working on is the encapsulation and delivery of both therapeutic and diagnostic agents.

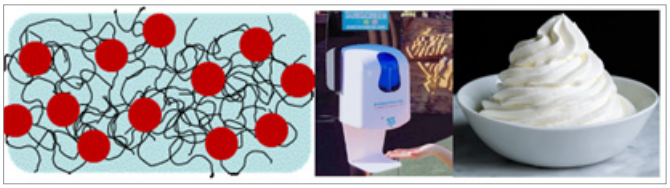
Shear-Induced Phase Inversion (SIPI) technology for green bioprocessing applications

Emulsion gels play a key role in daily life, eg cosmetics, sunscreens, pharmaceuticals and food products. Conventional processes in making emulsion gels involve the use of large quantities of unwanted chemicals. Our novel SIPI technology can produce emulsion gels using natural biopolymers without the use of unwanted chemicals.

Using SIPI technology, stable emulsions can be generated for food, dairy, pharmaceutical industries and agri-business. SIPI can also be used for emulsion-separation processes to enhance productivity in the oil industry.



Scanning electron microscopic images of ultrasonically synthesized chitosan microspheres used for the encapsulation of bioactives/flavours.



SIPI Technology can be used for making high quality emulsion gels.

Professor Brendan Abrahams

Professor Brendan Abrahams

- Crystal engineering
- Supramolecular chemistry
- Coordination polymers
- Molecular cages
- X-ray crystallography

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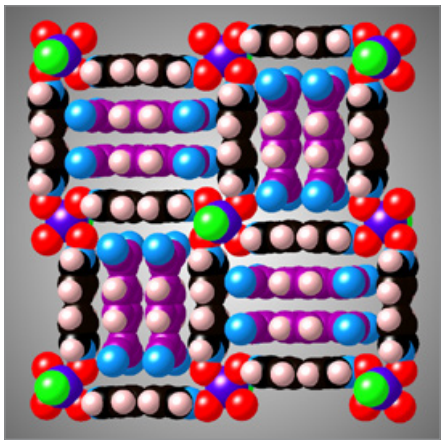
To use simple geometric and chemical principles to assemble molecular structures that exhibit unusual and technologically useful properties, such as electronic communication and adsorption behaviour.

Design, synthesis and properties of new materials

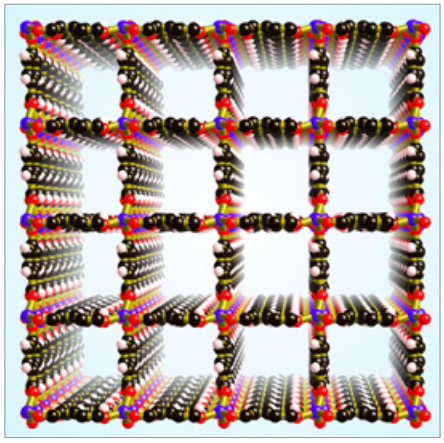
Our group is interested in linking molecular building blocks into discrete and polymeric structures using design principles based upon simple geometry and anticipated chemical behaviour. Some of the products are porous and have been tailored towards a specific adsorption application, whilst others are intended to exhibit electronic communication between molecular components. The research areas include:

1. Redox-active network materials
2. Porous coordination polymers
3. Hydrogen-bonded network materials
4. Molecular cages.

Much of the research is directed towards determination of molecular structure using single crystal X-ray diffraction. A wide variety of physical measurements are undertaken on the materials synthesized including gas adsorption and electrical conductivity. A major aim of our research is to rationalise the properties of the materials we generate in terms of the molecular structure and thereby establish structure-function relationships.



An iron-based electrically conducting network material.



A strongly adsorbing zinc-based coordination polymer.

Professor Evan Bieske

Professor Evan Bieske

- Molecular spectroscopy
- Mass spectrometry
- Molecular ions
- Astrochemistry
- Photochemistry

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We develop and deploy sensitive and selective techniques of our own device to probe exotic molecules postulated to exist in the interstellar medium and the terrestrial atmosphere, which may form the basis of new opto-electronic devices. The gas-phase vibrational and electronic spectra of these molecules help us address fundamental aspects of molecular structure, photochemistry and chemical reactivity, allowing us to identify molecules with potential technological applications and provide essential data for probing the molecular constitution of extraterrestrial regions.

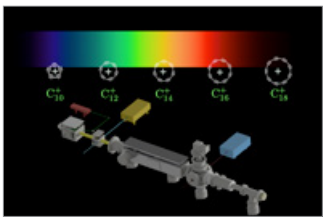
Our broad goal is to understand the properties and behaviour of charged molecules and clusters. Although molecular ions are ubiquitous, playing central roles in the chemistry of terrestrial and extraterrestrial systems, it is difficult to examine their intrinsic properties because they are difficult to isolate, as they normally interact strongly with other molecules. Our approach is to select and isolate ions in a vacuum environment where they are probed using light from tunable lasers. We integrate specialised mass spectrometers (that we build ourselves) with sophisticated laser systems to achieve extraordinary sensitivity and selectivity for our spectroscopic studies.

Spectroscopy of astronomically relevant molecular ions

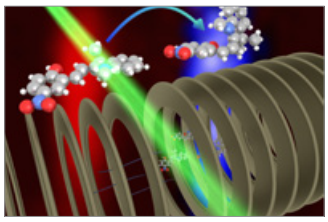
The regions between stars are not empty but rather are populated by a range of exotic molecules that have been identified mainly through radio astronomy. Our goal is to make and spectroscopically characterise new molecules in the laboratory and to measure their electronic and infrared spectra, which can then be compared with astronomical data to determine whether the molecules exist in space. Our current focus is on charged carbon clusters: species that include the molecule buckminsterfullerene (C60+). One of the fascinating (and challenging) aspects of the experimental studies is that smaller carbon clusters exist as chains, rings, fullerene and graphene structures. We have developed new techniques to form, separate and isolate the different isomers so that their unique properties can be experimentally unveiled, allowing us to assess whether they exist in interstellar space, and whether — like buckminsterfullerene — they possess useful optoelectronic properties.

Spectroscopy of shape shifting molecules

Molecules that change shape in response to the absorption of light are important in the visual apparatus of animals and in molecular photoswitches and motors. Understanding the way in which light causes molecular rearrangements is important for developing better molecular photoswitches and for understanding the light response of various biological systems. We have developed a new experimental approach for probing light-induced changes in molecular structure. The technique is an extension of ion mobility mass spectrometry, a method by which charged molecular isomers are separated according to their collision cross section with a neutral buffer gas: compact molecular ions travel more quickly through the buffer gas than extended ions. We deploy this approach to investigate fundamental photochemical processes, including trans-cis photoisomerisation, and photocyclisation and linkage photoisomerisation, in diverse molecules of biological and technological relevance.



Carbon rings absorb light across the visible region.



Photoisomerisation of charged molecular photoswitches in the gas phase.

Professor Colette Boskovic

Professor Colette Boskovic

- Inorganic chemistry
- Transition metals
- Rare earths
- Molecular materials
- Magnetochemistry

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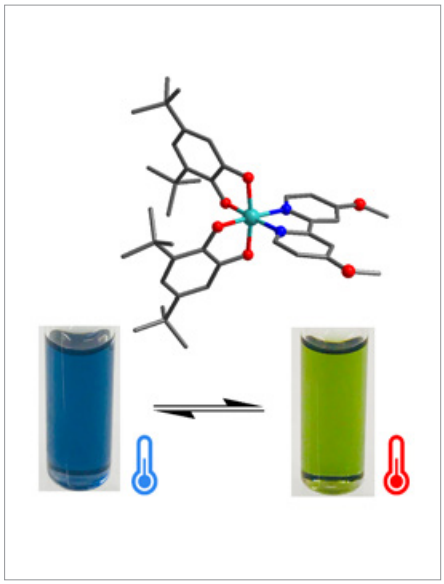
The majority of elements in the periodic table are metals, and many of these are abundant in Australia. Compounds of metals exhibit tremendous chemical versatility and a range of properties, for example the blue colour of copper salts versus the red of iron rust. These properties are amenable to control by chemists and can be harnessed in a range of advanced technologies. We seek to design and make metal-based molecular materials for future applications, including in sensors, display devices, high density data storage, quantum computing and molecular electronics or spintronics.

Smart molecular materials

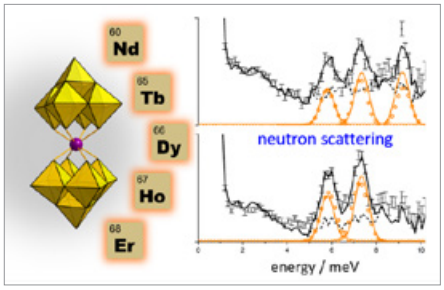
Molecular materials that can be interconverted between two distinct forms are of interest for future applications as sensors, in display devices, and for molecular electronics and spintronics. We are interested in smart materials based on transition metals like cobalt and iron, which can be interconverted between two or more forms by heating and cooling or exposure to light. We are presently focusing on developing computational methods to identify new candidate molecules to guide our synthetic targets in the laboratory. We have also developed smart molecules that can act as three state switches for more complex switching applications.



Smart molecular material.

Rare earth chemistry

Rare earth metals are essential components of many devices, including magnets, phosphors and lasers. Australia has significant untapped reserves of many of these elements, which have only recently begun to be developed. We are targeting compounds of rare earth metals with ligands that can be easily oxidised or reduced to develop new molecular materials with switchable magnetic and luminescence properties.



Rare earth chemistry.

Single-molecule magnets

While conventional bulk magnets are based on interactions between different metal ions, single-molecule magnets are species that exhibit retention of magnetisation at low temperature due to molecular properties. A single magnetic molecule could act as the smallest possible unit of magnetic memory, affording significant enhancements in high density magnetic data storage. Single-molecule magnets also exhibit magnetisation quantum tunnelling and are of interest as qubits for quantum computers.

Dr Brad Clarke

Dr Brad Clarke

- Pollution
- Emerging contaminants
- PFAS
- Microplastics
- Analytical chemistry

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I am advancing the science of emerging contaminants through multi-disciplinary research that applies state-of-the-art analytical technologies to increase our understanding of the occurrence, fate, exposure, risk, hazards and remediation strategies of legacy and emerging contaminants.

Contamination of the environment with anthropogenically produced chemicals is one of the most serious environmental issues facing contemporary society. While synthetic chemicals are indeed essential for modern society, some can be particularly problematic. The worst of these pollutants:

- Biomagnify through the food chain, accumulating in humans and wildlife
- Cause negative health impacts including cancer, reproductive health problems, impaired immune function and neurodevelopmental impairment
- Are detected frequently in all environmental compartments (air, water, soil, biota) across the globe, including 'pristine' locations far from known point sources, where they can persist for decades or even longer
- Can be difficult to remediate or remove by natural processes from environmental matrices due to a combination of unique chemical properties and high cost of treatment.

There are over 163 million unique chemical compounds registered in the Chemical Abstract Service (CAS) database and over 147,000 of these are routinely used for industrial applications. For many new recently discovered emerging contaminants, we have no information on their persistence, environmental behaviour and/or toxicology. Current global approaches to chemical management involve the constant introduction of new chemicals with little thought for their potential impact on society and the environment. In fact, we are now engaged in an experiment involving all of humanity, where we are exposed to a mixture of thousands of chemicals in our daily life. Therefore, it is essential to conduct research that increases our scientific understanding of a wide range of organic pollutants, including how they cycle through the environment and the toxicological impact resulting from exposure.

Sampling the environment.

Professor Paul Donnelly

Professor Paul Donnelly

- Inorganic chemistry
- Bioinorganic chemistry
- Metal ions in biology and medicine
- Metal ions in catalysis
- Coordination chemistry

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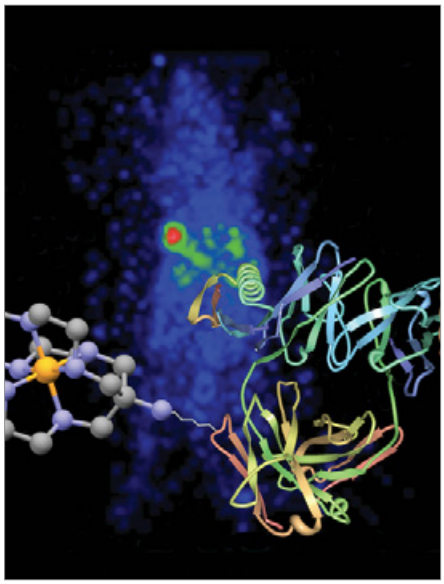
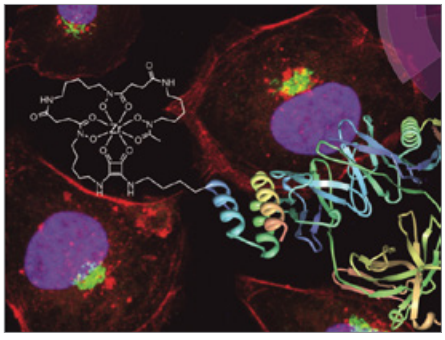
The group focuses on synthetic inorganic and organic chemistry to make new metal-containing compounds with potential applications in biology.

We are interested in the application of coordination complexes and metal-based compounds as diagnostic and therapeutic agents. Exploratory synthetic coordination chemistry and the design of new metal complexes underpins all of our research. We also investigate the roles of metal ions in cellular biology, with a particular focus on chemical aspects of neurodegeneration. Our multidisciplinary research involves inorganic and organic synthesis, followed by characterisation utilising a wide range of analytical techniques, including multinuclear NMR, electronic spectroscopy, EPR spectroscopy, mass spectrometry, HPLC, electrochemical techniques and X-ray crystallography.





Dr Alex (Xiaofei) Duan

Dr Alex (Xiaofei) Duan

- Chemical analysis
- Separation
- Chromatography
- Materials
- Hyphenation

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My research focuses on applications of advanced separation and analytical technologies to investigate materials recycling, such as used catalysts and polymers. In particular, the scientific study of green processes will address many environmental concerns in the recycling industry. Hyphenation technology for chemical analysis provides economical investigation of synthetic and biopolymer materials and elemental speciation such as arsenic and selenium, which have significant environmental impact.

Hyphenation technology for chemical analysis

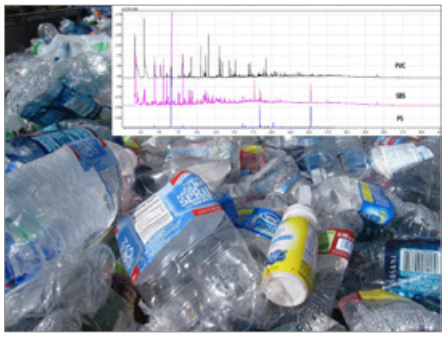
Hyphenation technology employs a combination of analytical tools, and is used in areas such as liquid chromatography atomic fluorescence spectroscopy (LC-AFS) for Arsenic (As) and Selenium (Se) speciation. Another important technology is pyrolysis gas-chromatography mass spectrometry (Py-GCMS), a technology widely applied in the investigation of plastics, rubbers and biopolymers. I use these technologies to provide better analytical insight and solutions for research and industry communities.

Advanced separation technology

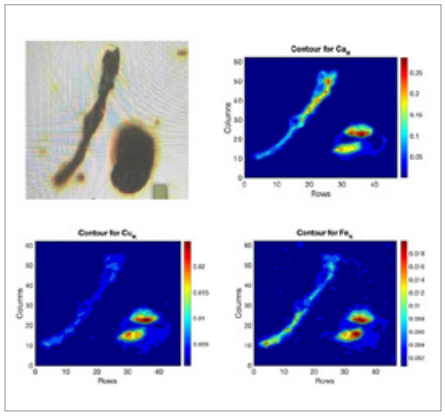
Hydrometallurgy is a primary technique employed in the recovery of catalytic metals in automobile and electronic industries, offering high purification and selectivity with promising recovery yield. A key application is the recycling of platinum group metals (PGMs) from spent catalytic converters (SACs). PGMs, including platinum, palladium and rhodium, are used to reduce the emission of hazardous gases CO and NOx. They exhibit numerous unique chemical properties, such as high stability and selectivity, high corrosion resistance and catalytic activity. However, PGMs are scarce. Thus, recycling them from secondary resources, particularly SACs, is significant work. I aim to use advanced membrane separation in hydrometallurgy to provide greener, more efficient recovery of PGMs.

Medicinal cannabis

Medicinal cannabis research is an emerging topic around the world. However, analysing cannabis can be very challenging. The regulation, research licensing, sample handling and preparation remain unclear. In addition, there are many factors that affect the growth of cannabis materials and relevant products. I aim to extend my initial research at Synchrotron, which investigated elemental localisation and distribution. This elemental study may hold the key to the production of high-grade cannabis materials.



Plastic identification for recycling.



Elemental localisation.

Professor Ken Ghiggino

Professor Ken Ghiggino

- Lasers
- Photochemistry
- Spectroscopy
- Polymers

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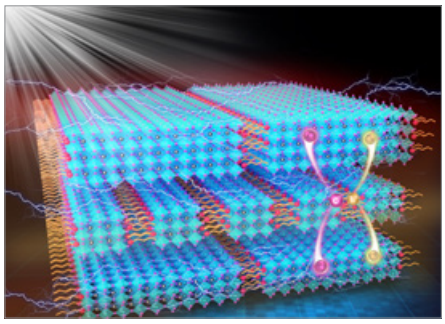
Harnessing light-driven chemistry will make a major contribution to resolving the world's future energy needs through the development of more efficient solar cells and solar fuels. Our research seeks the fundamental understanding required to develop new materials and devices that use light more efficiently and productively for the benefit of society.

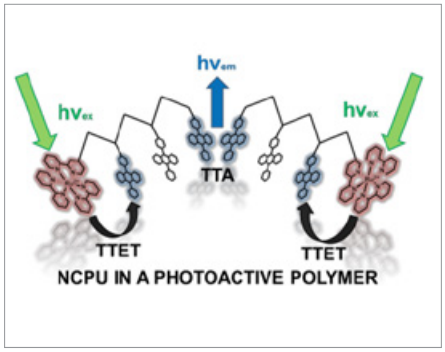
Photochemistry

Light-driven chemistry underpins photosynthesis, medical phototherapy, solar degradation of materials, and solar-driven renewable energy systems. Our research involves the development and application of advanced laser-based spectroscopic techniques to understand the initial steps of photochemical processes in both biological and man-made materials. These techniques include ultrafast spectroscopy, luminescence, and single-molecule fluorescence imaging.

The instrumentation available in our laboratories allows the observation of photon-initiated events occurring on the femtosecond time scale and at spatial resolutions of less than a micron. Current projects involve characterising new solar cell materials that can be printed onto flexible, lightweight plastic substrates; the development of new solar harvesting and light-concentrating devices; and the imaging of light-induced processes in single molecules.



Sandwich structure of a 2D perovskite solar cell film.



Light energy upconversion process in a synthetic polymer.

Dr Marcus Giansiracusa

Dr Marcus Giansiracusa

- Lanthanoid
- Electronic structure
- Computational chemistry
- Magnetism
- Spectroscopy

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I study single-molecule magnets (SMMs) for applications in data-storage and spintronics (emerging electronic technology), or as qubits (the basic information units in quantum computing).

Crystal field splitting in Erbium and Ytterbium(III) molecules

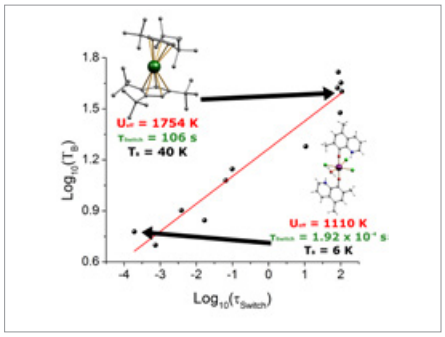
Lanthanoid metals have properties critical for specific applications. SMM research has focussed on Dy(III) complexes. In contrast, the Melbourne Magnetometry Laboratory is investigating Er(III) and Yb(III) complexes, using neutron-scattering spectroscopy and the Spartan computational platform, to create a stronger theoretical framework for predicting the properties of SMMs.

Relaxation times extracted from inelastic neutron-scattering spectroscopy (INS)

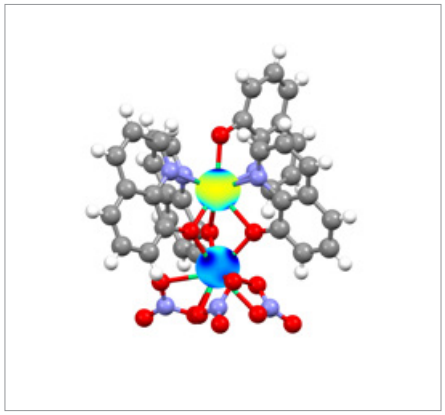
Understanding novel relaxation pathways in SMMs or qubits is essential to enhance their properties for applications. A magnetoelastic coupling relaxation model can be applied to data from older INS studies of qubit candidate complexes, even if relaxation dynamics was not the original focus.

Magnetic fingerprint for ochre samples

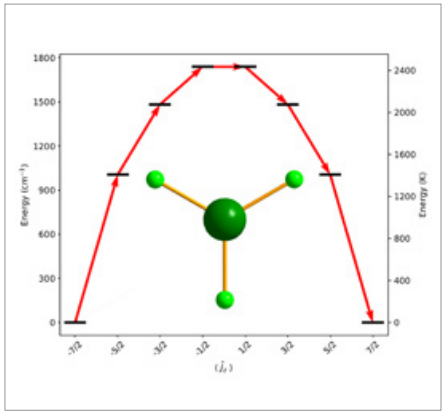
We magnetically characterise ochre samples from around the world, using the MPMS3 SQUID Magnetometer, to increase understanding of materials movement by ancient civilisations.



Studying trends in single-molecule magnets to identify magneto-structural correlations.



Understanding the impact of ligands on the electronic structure of lanthanoids.



Using ab initio calculations to understand the stabilisation of spin-orbit coupled states, wavefunction information and transition probabilities.

Associate Professor Lars Goerigk

Associate Professor Lars Goerigk

- Theoretical quantum chemistry
- Computational chemistry
- Density Functional Theory
- Noncovalent interactions
- Thermochemistry of ground and excited states

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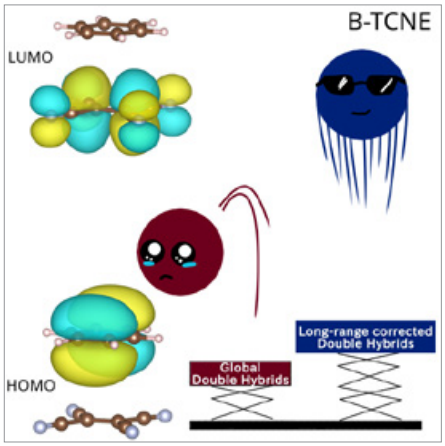
It has always fascinated me that we can, in principle, solve chemical problems without having to go to the lab. In practice, it is impossible to solve the related quantum-mechanical equations for real-life chemical problems, but the field's strength stems from the development of robust approximations that yield results with surprising accuracy. I hope to be able to contribute towards developing even more accurate approximations that allow us to reliably predict new experiments before they are conducted.

Our research revolves around the exciting field of theoretical and computational quantum chemistry, which is the description of electrons in chemical systems by evoking the laws of quantum mechanics. Our interests comprise the development of new quantum-chemical methods, and collaborative applications to organic, inorganic, physico or biochemical problems. Some of our research highlights include: enabling more efficient and accurate computational treatments of chemical problems; developing some of the currently most accurate computational methods for the treatment of electronic excited states, which enable improved computational protocols for the simulation of problems related to sustainable power generation; and closing the communication gap between method developers and chemists that rely on pairing computational methods with their experiments. We developed new guidelines and recommendations that make such computational endeavours more reliable.

Theoretical/computational chemists do not wear lab coats or need bench space. Our computers are our lab.



This cartoon was used for a recent article on some of our newly developed computational methods. Those methods outperform older ones and allow the treatment of processes that involve electrons that travel relatively long distances from one part of a chemical system to another. The accurate modelling of such processes is, for instance, important for the development of more efficient solar cells.

Dr Christopher Hall

Dr Christopher Hall

- Photochemistry
- Ultrafast spectroscopy
- Multi-dimensional electronic-vibrational spectroscopy
- Ultrafast vibrational spectroscopy

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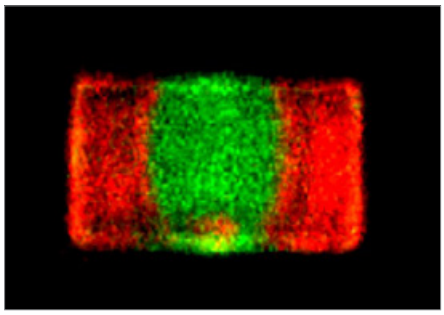
Progress in science can often be made by approaching long-standing problems from a new perspective. We seek to employ the most advanced laser-based spectroscopic techniques to provide new insight into problems where the conventional tools provide limited information. I am interested in photoactive systems and systems where vibrational spectroscopy can provide unique insight, including materials for solar and device applications, inorganic or organic electronics, fluorescent probes, optogenetic proteins, molecular motors, protein/molecular wires for charge-transfer, photocatalysis, photoactive biochemical systems and drug-target interactions.

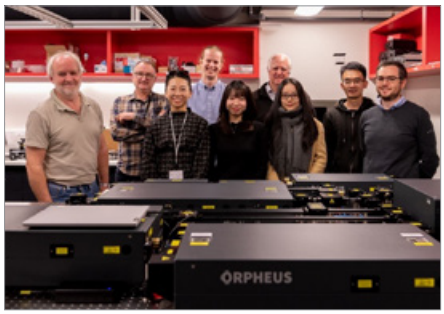
Electronic-vibrational spectroscopy: A new probe for structure and function

The generation of useful chemical states with light is central to research efforts in emerging technologies, including next-generation photovoltaics, bioelectronics, optogenetics and photocatalysis. Developing tools that can identify and quantify the fundamental interactions that participate in light-driven chemical reactions is critical for improving the performance of these systems.

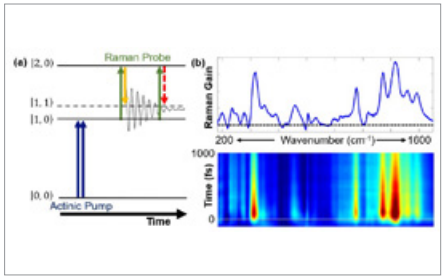
The leading methods for studying excited-state reaction pathways in fast photochemical systems are based on ultrafast laser spectroscopy. Despite 40 years of progress, identifying and quantifying competing reactions in photochemical systems remains a major challenge. To tackle this problem, we seek to combine ultrafast electronic and vibrational spectroscopies to open new avenues for spectroscopic investigation of photochemical systems. The techniques we are developing will provide sensitivity to the molecular structure of selected excited states and the ability to separate reaction pathways in order to assign the role played in excited-state processes. This new level of detail is expected to profoundly enhance our understanding of energy and chemical conversion in complex photochemical systems.



Scanning confocal microscope image of a single mixed-halide perovskite crystal showing emission from regions with different material compositions.



The ultrafast spectroscopy group, and the brand-new laser system.



Femtosecond Stimulated Raman Spectroscopy (FSRS). (a) The photochemical reaction is initiated by the actinic pump pulse. The excited-state structure is probed by the stimulated resonant Raman probe. (b) Example spectrum (top) and dynamics (bottom) of a dark excited-state for a molecular motor.

Dr James Hutchison

Dr James Hutchison

- Solar harvesting materials
- Trace (bio)molecule sensing
- Photochemistry
- Molecular polaritons
- Surface plasmon photonics

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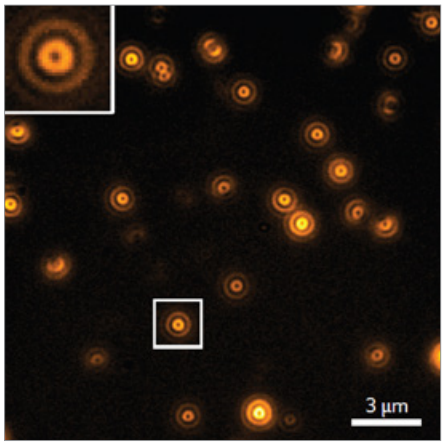
Controlling energy flow within and between molecules is one of the grand challenges of molecular science. This control allows one to concentrate light energy for solar harvesting and optical sensing and to direct thermal energy for site-selective chemistry. By texturing materials on the scale of the wavelength of light we can establish unique tools to assert such control, potentially uncovering new avenues for light-to-chemical energy conversion, photocatalysis, and trace molecular sensing.

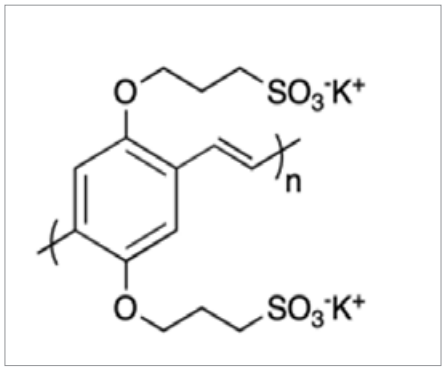
Novel solar harvesting devices

The transfer of energy between molecules after absorption of light is crucial to the efficiency of natural photosynthesis but also for the development of organic optoelectronic devices, including organic photovoltaics (OPVs) and luminescent solar concentrators (LSCs). Normally, energy transfer between molecules is efficient over distances of only a few nanometres, requiring multiple hopping events to transfer over macroscopic distances in devices. In the past decade, however, it has been shown that when molecules are placed inside mirror cavities (as simple as two metal films), multiple interactions between the molecules and light bouncing between the mirrors leads to highly delocalised states, or molecular polaritons, which may allow energy transfer over 100s of nanometres and increase the efficiency of light-harvesting devices.

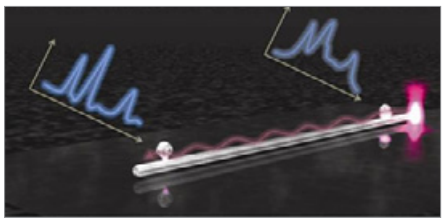
Trace (bio)molecule sensing

When light is shone on metal nanoparticles, the light can be trapped at the metal surface and travel along it. As the light is 'concentrated' at the surface, its intensity is enhanced over a billion times (this phenomenon is known as a 'surface plasmon'). If a molecule is placed at the surface of the particle, it can undergo strongly enhanced fluorescence, photochemistry, and Raman scattering. In this way, one can detect trace amounts of a molecule of interest. We are currently targeting short strands of RNA, microRNA, and other biomarkers for diseases such as cancer, towards developing sensors for early diagnosis.





Energy transfer in light-harvesting polymers studied by fluorescence imaging.



Schematic of light captured by, and propagating along, the surface of a silver nanowire towards molecular detection.

Professor Craig Hutton

Professor Craig Hutton

- Peptide synthesis
- Synthetic methodology
- Organic synthesis
- Chemical biology

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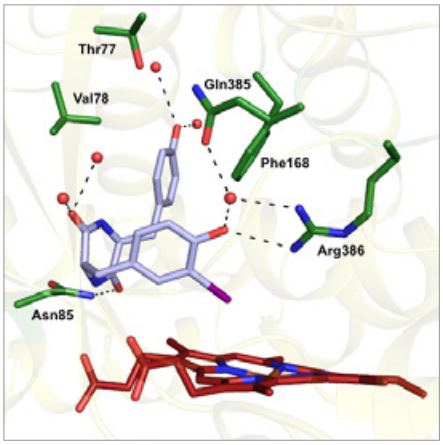
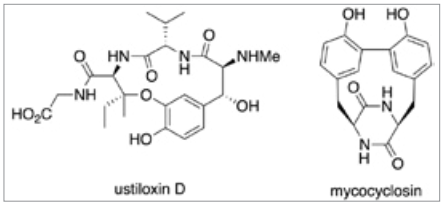
Our goal is to develop new chemical reactions to enable the synthesis of peptides and proteins for use as therapeutic agents. Biosynthesis of peptides and proteins follows specific pathways to ensure fidelity; using new chemical methods we can expand the repertoire of molecules that can be constructed and exploited to understand and treat disease.

Our expertise is in the areas of amino acid, peptide and protein chemistry. Our research areas include the development of new synthetic methods for peptide and protein synthesis, the total synthesis of complex cyclic peptides natural products and the development of radiolabelled peptides for the imaging of cancer.



Novel methods for peptide synthesis and ligation

We are investigating novel synthetic methods for forming amide bonds through the development of a silver-promoted coupling of thioamides and carboxylic acids. We recently employed this methodology to develop a novel peptide cyclisation process that avoids common problems such as cyclodimerisation and epimerisation.

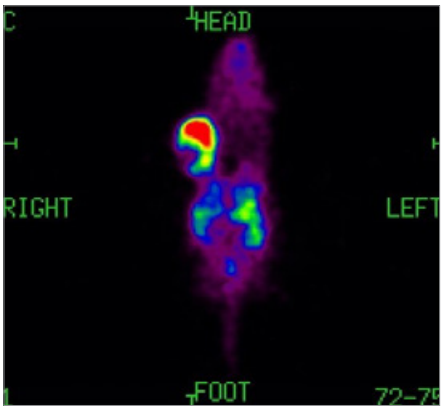


Synthesis of cyclic peptide natural products

We design new, efficient synthetic routes to biologically active complex cyclic peptides such as ustiloxin D and mycocyclosin. Novel strategies for the stereoselective synthesis of unusual amino acids and efficient preparation of the side-chain cross-links present in these peptides are critical to their ultimate synthesis.

Radiolabelled peptides for cancer imaging

We are developing new methods to incorporate the 18F-radionuclide into amino acids and peptides for imaging cancer by positron emission tomography (PET).



Associate Professor Guy Jameson

Associate Professor Guy Jameson

- Iron
- Enzymology
- Mossbauer
- EPR
- Kinetics

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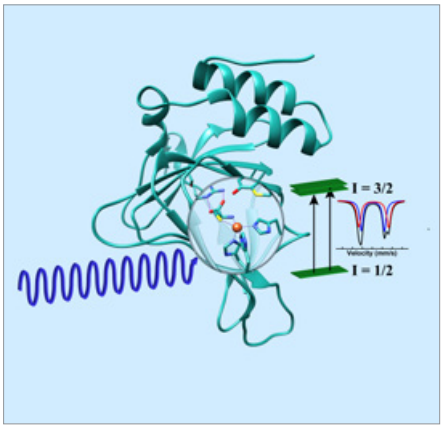
My research into biological systems brings together my expertise in spectroscopy and kinetics of proteins and small molecules and aims to understand the chemical basis of disease. Through studying how enzymes work at the molecular level we can understand how enzyme malfunction contributes to disease progression.

Iron is the most abundant element on earth and one of the most abundant in the earth's crust. Due to its high availability before the introduction of oxygen-producing organisms, it has been suggested that life started with iron (Günter Wächtershäuser). This also explains why iron-based chemistry lies at the heart of all life. Iron has a broad redox chemistry, and therefore it is used in oxidation catalysis and bioenergetics as well as acid-base reactions.

My research into enzyme mechanisms involves molecular biology and protein purification as well as physical, chemical, spectroscopic and kinetic characterisation techniques. Our group aims to understand how iron-oxygen reactivity is attained and regulated in the body. Through this, we can develop knowledge that is essential for understanding both physiological and pathophysiological processes, increasing knowledge of iron-oxygen reactivity in both chemistry and biology.



We study iron containing metalloenzymes using an iron specific nuclear spectroscopy called Mossbauer spectroscopy.

Associate Professor David Jones

Associate Professor David Jones

- Organic semiconductors
- Organic solar cells
- Catalysis
- Singlet fission
- Materials synthesis and characterisation

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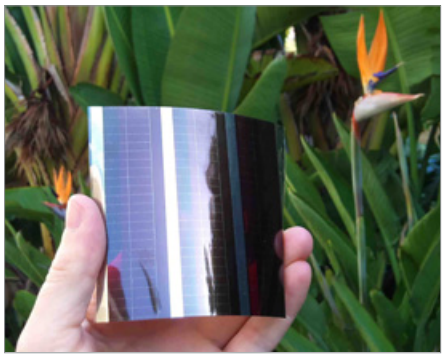
The key driver of my research is to lower the cost of solar power to enhance and underpin all other technologies. A significant reduction in cost will enable PV to be specifically deployed to 1. Drive storage systems, ie pumped hydro, super capacitors, batteries and so on, 2. Act as an enabler to drive the 'internet of things', such as self-powered sensors/displays, or 3. Drive chemical reactions, such as water splitting for hydrogen generation and in our modern world provide power for remote refrigeration for vaccine storage.

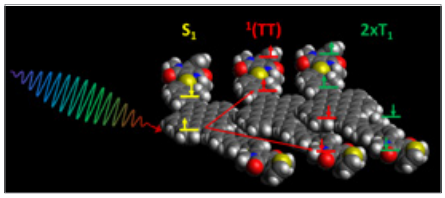
I am a Research Group Leader developing high performance organic electronic materials for large area printed solar cells and their translation to large area printed solar cells (**www.organotronics.com**). I have developed new classes of high-performance materials, including p-type organic semiconductors with a high temperature nematic liquid crystalline phase and exceptional materials properties, and new classes of Singlet Fission materials supporting quantum coupled states for enhanced solar cell efficiency. I run an advanced organic synthesis laboratory with materials characterisation tools along with a new integrated glovebox for solar cell device assembly.

Current research programs are:

- High performance p and n-type organic semiconductors (OSCs) for organic solar cells (organic photovoltaics OPVs)
- Translation to large scale printed OPVs
- Thermally activated delayed fluorescent (TADF) materials for OPVs
- Molecular OSC materials for singlet fission, and
- Nanoparticle composites as photocatalysts for direct reduction of carbon dioxide to solar fuels.



Printed solar cell.



Singlet fission: one photon to two excited states.

Dr John Karas

Dr John Karas

- Peptide and protein synthesis
- Synthetic methodology
- Medicinal chemistry
- Enzymes

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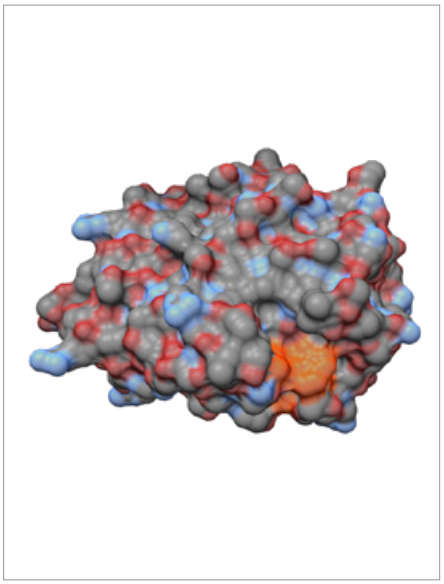
My research seeks to develop new chemical methods that enable the efficient preparation of biologically active peptides and proteins at scale. A key aim is to improve the thermal and chemical stability of proteins and enzymes for therapeutic and industrial applications.



Enhanced chemical protein synthesis

Chemical protein synthesis enables the preparation of important biomolecular targets to answer biological questions of significance. Its key advantage over recombinant protein expression is the ability to site-specifically incorporate post-translational modifications, chemical probes and non-native amino acids with high precision. Access to mirror image proteins is also possible, which are useful research tools for X-ray crystallography and peptide drug discovery.

Currently, the scope of chemical protein synthesis is limited to the production of small proteins since larger targets are difficult to obtain in good yield and at high purity. Our research is focused on developing new amino acid precursors to enhance the assembly of proteins. This will, in turn, enable access to larger targets of interest, such as therapeutic proteins, receptors and enzymes.

Next generation insulin therapeutics

Insulin replacement therapy is essential for the effective management of type 1 diabetes. But despite the relative success of subcutaneously administered basal/bolus insulin dosage regimens in controlling blood glucose levels, significant challenges remain to optimise treatment, such as: (i) increasing therapeutic compliance; (ii) improving glycemic control; and (iii) enhancing formulation stability. Therefore, we are developing a new generation of glucose-responsive insulins, which only activate when blood-glucose levels are elevated. Hyper-stable analogues are also under investigation, which will be ideal for use in insulin pumps and oral formulations.

Hyper-stable enzymes

Enzymes enable precise chemical transformations of various substrates and are commonly used in the food, beverage and chemical manufacturing industries, to name a few. However, enzymes are typically susceptible to thermal and chemical denaturation, whereby their native tertiary structure can be altered to a non-active state. This limits their utility, as only ambient temperatures and mild reaction conditions can be used. Therefore, we are investigating new synthetic methods for modifying these biocatalysts to address the stability issue, which will lead to recyclable enzymes that can be used for a broader range of applications.

Dr Ivanhoe Leung

Dr Ivanhoe Leung

- Enzymology
- Biological chemistry
- Inhibitor discovery
- NMR spectroscopy
- Protein-ligand interactions

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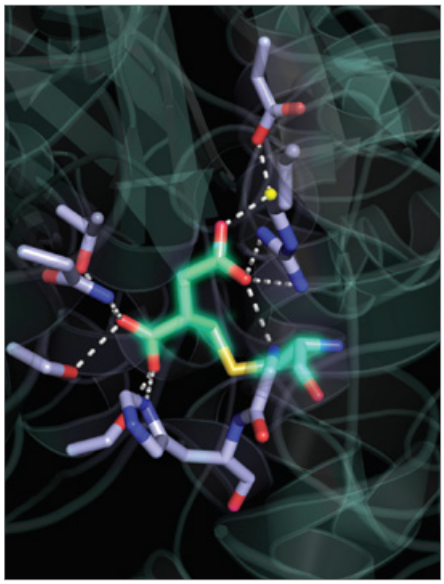
We aim to utilise our knowledge of protein structure and enzyme mechanisms to help solve some of the world's most urgent challenges. The Leung Research Group focuses on the enzymology that involves protein function modulation. We apply a range of biophysical, chemical biology and structural biology techniques to enable our discoveries.

Metabolic regulation of protein functions

The ability to maintain homeostasis is critical to all forms of life. One mechanism through which this is achieved is the fine-tuning of cellular enzyme activities. In our group, we study how posttranslational modifications and metabolites affect the structure, activity and function of proteins and enzymes. These allow us to understand how different biochemical pathways signal and interact with one another to maintain stability in response to stress conditions. We are currently studying the enzymes that are involved in the regulation of carbon metabolism in Mycobacterium tuberculosis to understand how the pathogen survives inside the infected host with limited nutrients. Another system that we are studying is the plant ethylene-forming enzyme. We are presently investigating the mechanisms and structures of the different enzyme isoforms with a view to developing a detailed understanding of their roles in plant growth and development.



Inhibition of the Mycobacterium tuberculosis isocitrate lyase by the human macrophage metabolite itaconate.

Enzyme technology for bioremediation

Enzymes are highly efficient catalysts that speed up chemical transformations under mild conditions. In our group, we study how we could harness the incredible catalytic prowess of enzymes as green biocatalysts to degrade environmental pollutants. We are especially interested in laccases, a class of multi-copper oxidase enzymes that catalyse one-electron oxidation of aromatic amine and phenolic substrates. Currently, we are studying how laccases mediate the degradation of organic pollutants at a molecular level to understand their mechanisms of catalysis. We also characterise the degradation products under different reaction conditions to investigate plausible degradation pathways.

Inhibitor discovery strategies and applications

The ability to modulate the activity of enzymes using natural or synthetic compounds has enormous potential in areas such as medicine. An important step in the early stages of inhibitor development is the identification and characterisation of ligands that bind to the target. Our laboratory specialises in the application of biophysical techniques, especially NMR spectroscopy, for ligand screening and to study protein-ligand interactions and enzyme inhibition. A current interest is the development of inhibitors for lipid A phosphoethanolamine transferases. Such compounds have potential to be used as adjuvants to reverse bacterial resistance to polymyxins, a class of last-line antibiotics to treat multidrug-resistant infections.

Professor Megan Maher

Professor Megan Maher

- Metals in biology
- Structural biology

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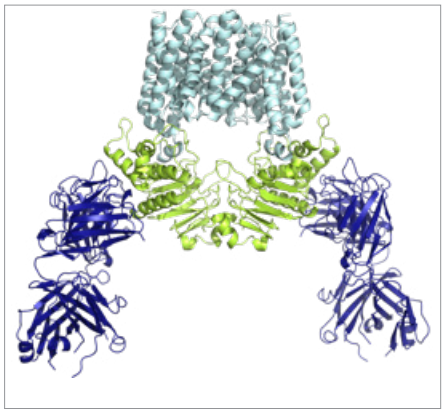
I seek to revitalise the current understanding of the roles of trace elements in biology by providing a holistic view of their acquisition and balance in cellular systems.

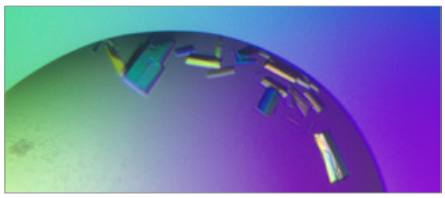
Trace elements such as iron, copper and zinc are required nutrients for all forms of life, but their essential nature is offset by their potential for toxicity. In all cells, the acquisition and balance of trace elements is finely tuned, as dysregulation leads to disease. For example, imbalances have been implicated in conditions such as neurological disorders (Alzheimer's disease, Parkinson's disease and prion diseases), trace elements play a critical role in infection as agents of innate immunity, and metal-based medicines (eg platinum) are used as chemotherapeutic agents.

A fundamental understanding of trace element homeostasis is a key component of a holistic model of cellular behaviour. Ground-breaking research in the field over the past 20 years has established that trace elements are managed by exquisitely tuned protein-based systems that function in synchronicity to manage cellular nutrient uptake, efflux and trafficking. However, most research on these systems has been fragmented, focusing on isolated aspects and properties of these networks. Consequently, our appreciation of the role of metals in biology remains crude. My work uses structural biology (particularly X-ray crystallography) to define the architectures of these protein systems and applies this structural information to unravel how these complex systems function. By coupling these insights with functional characterisations through cell biology and biochemical and biophysical techniques, I am constructing a comprehensive vision of biological trace element homeostasis. Specific projects currently under investigation in my laboratory include:

- Cellular metal homeostasis: how trace elements are balanced within biological systems
- Metal transport across membranes: structures and functions of integral membrane protein transporters
- Metals in the mitochondria: mechanisms of assembly of mitochondrial complexes relevant to mitochondrial disease
- Electron transfer within and between protein metal sites.



The structure of a bacterial metal transport protein that is a target for novel antibiotic design.



Protein crystals are not only beautiful, but are the basis for determining protein structure.

Professor Paul Mulvaney

Professor Paul Mulvaney

- Physical chemistry
- Materials science
- Spectroscopy
- Nanocrystals
- Solar energy

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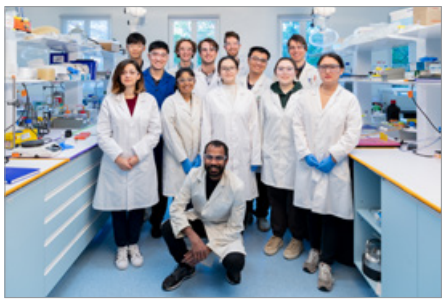
excitonscience.com

Our goal is to discover new materials that can help Australia transition to a sustainable energy future.

The Centre of Excellence in Exciton Science is led by the School of Chemistry. Our main focus is on nanoscale materials (quantum dots, quantum rods, quantum wells), and the way they interact with light. Our group also makes prototype devices to test and measure the properties of new materials such as QLEDs, solar cells, transistors and sensors.

We collaborate with other Chemistry groups (Wong, Ghiggino, Smith, Boskovic, Goerigk), as well as external partners including CSIRO, Australian Synchrotron, DSTG, and the Reserve Bank.

Quantum dots are small semiconductor crystals just 1-20nm across. Their size controls their optical properties. The image shows luminescence from cadmium selenide crystals, ranging in size from 1-6nm.



The Nanoscience Laboratory is part of the ARC Centre of Excellence in Exciton Science.

Professor Richard O'Hair

Professor Richard O'Hair

- Mass spectrometry
- Homogenous catalysis for organic synthesis
- Non-targeted metabolism of exogenous substances

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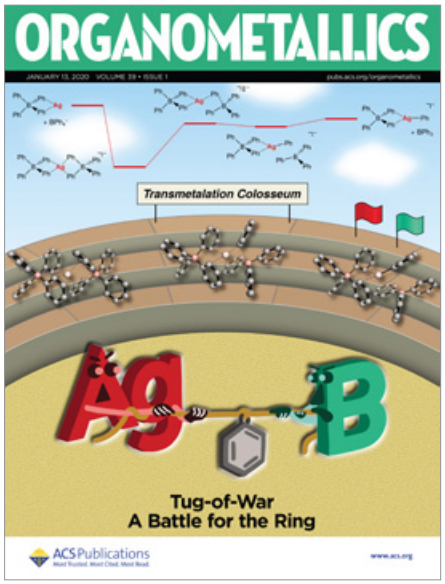
Our mission is to study reactive intermediates, understand novel structure and bonding motifs, design new catalysts and invent new reactions. We blend gas-phase experiments, DFT calculations and solution phase chemistry to achieve this.

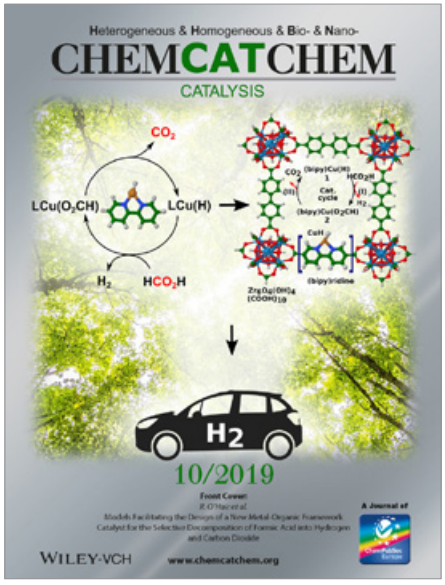
Generating a wide range of inorganic, organometallic and organic ions using electrospray ionisation (ESI), we then take advantage of multistage mass spectrometry (MSn) techniques to unmask reactive intermediates (via collision induced dissociation, CID) so that we can examine their reactivity via ion-molecule reactions (IMR). Knowledge gained is translated to the condensed phase.Fundamental and applied mass spectrometry

Mass spectrometry (MS) is a powerful tool to analyse a wide range of molecules and to study fundamental chemistry in the gas phase. Research in my group is focused on the use of advanced MS techniques and molecular modelling methods to explore contemporary problems in chemistry and at the chemistry/biology interface. I am particularly interested in understanding the mechanisms of reactions widely used in synthesis, including organometallic reactions and transition metal catalysed reactions. Another key area is the development of radical based methods for the analysis of biomolecules via MS.

Our applied MS work has involved identification of small bioactive molecules and the revitalisation of the Twin Ion Method to study metabolism of exogenous small molecules (eg insecticides or drugs) in animal models in vivo. These studies are often carried out in collaboration with workers in the USA, France and Germany and with collaborators at the Bio21 Molecular Science and Biotechnology Institute.



Recent cover art on developing understanding of a key class of reactions.



Recent cover art on developing a new class of catalyst for release of hydrogen.

Dr Charlotte Petersen

Dr Charlotte Petersen

- Computational chemistry
- Glass
- Nonequilibrium systems
- Molecular dynamics simulations
- Statistical mechanics

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I aim to understand the astoundingly complex behaviour of some everyday materials using computer simulations and statistical mechanics theory. I apply this approach to a range of amorphous and frustrated materials, glassy liquids, and flow through porous materials.

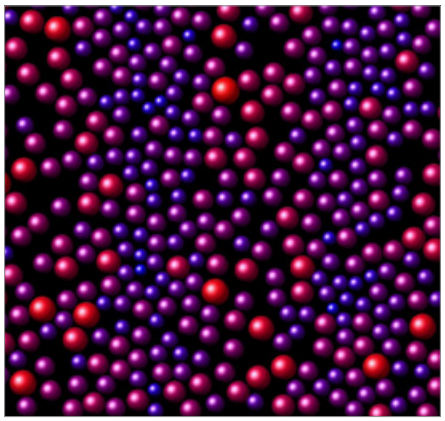
Molecular dynamics simulations of glass

At large scales, glass behaves like a solid, yet its microscopic structure is disordered like a liquid. This makes it difficult to predict the mechanical properties of new glasses, so they are designed through trial and error. To address this problem, I classify the structure of a glass material by how much the atoms vibrate, measured by the degree of blurring in the material's diffraction pattern (as is done routinely for crystals), and link this to the glass's macroscopic properties via computer simulations.

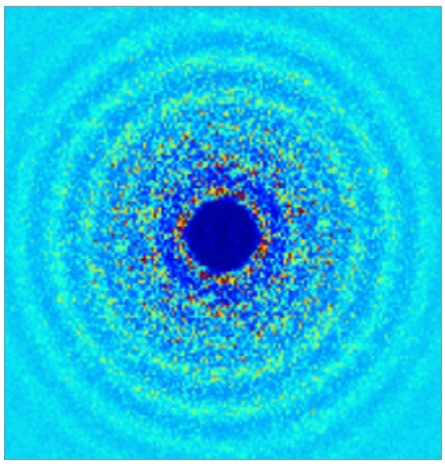
Future research plans

Violations of the Second Law of thermodynamics

Understanding how new miniaturised technologies such as nanobatteries and molecular machines violate the Second Law of Thermodynamics is essential to rational design. Recent theory is closing this gap but is challenging to apply experimentally. By studying artificial spin ice, a new material designed for easy observation of thermal fluctuations, I aim to link theoretical predictions to measurements.



Snapshot from a molecular dynamics simulation. These simulations allow us to follow the motion of individual particles. By monitoring the motion of particles in a glass, we can measure the vibrations.



Simulated diffraction experiment on a glass. Although this diffraction pattern is too noisy and complex to measure detailed structural information directly, by measuring how it changes with temperature we can infer how much the particles are vibrating.

Associate Professor Anastasios Polyzos

Associate Professor Anastasios Polyzos

- Synthetic organic chemistry
- Flow chemistry
- Catalysis
- C-H activation
- Palladium chemistry

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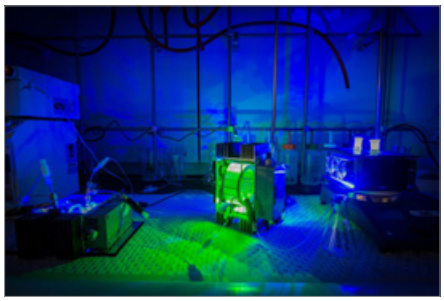
Research in our laboratory is focused on the discovery of methods in synthetic organic chemistry. These methods will enable the direct synthesis of biologically active molecules with the enzyme-like efficiency observed in nature and furthermore will lead to the sustainable manufacturing of new pharmaceuticals.

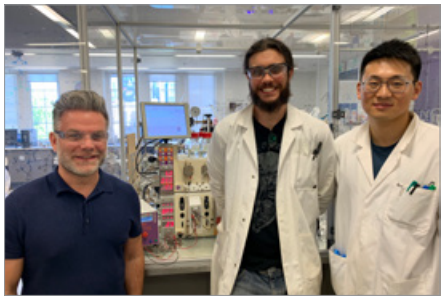
We discover novel methodologies and technologies for organic synthesis. Our group harnesses catalytic reactions and flow chemistry to achieve the sustainable synthesis of complex organic molecules with enzyme-like efficiency.

Key interests include:

- Visible light photoredox catalysis
- Direct C-H activation with high oxidation state palladium catalysis
- Flow chemistry
- Total synthesis of natural products and medicinal chemistry.



A continuous flow photo chemistry reactor at the School of Chemistry. Image credit: UoM Image Bank.



From left to right: Dr Anastasios Polyzos and PhD students Jose Forni and Xiaocong Guan from the School of Chemistry. Image credit: Anastasios Polyzos, UoM.

A photoredox chemical reaction illuminated by light emitting diodes. Image credit: Anastasios Polyzos, UoM.

Professor Gavin Reid

Professor Gavin Reid

- Analytical chemistry
- Biochemistry
- Mass spectrometry
- Molecular 'omics'
- Chemical analysis

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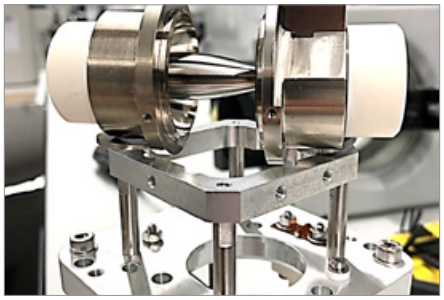
The structural diversity and complexity of biological and chemical molecules presents a significant challenge to their comprehensive identification and characterisation. We aim to address these challenges through the development of novel analytical measurement strategies involving cutting-edge mass spectrometry instrumentation and methods.

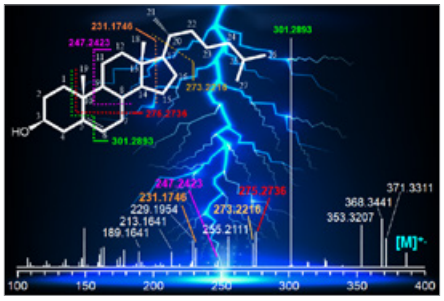
Bioanalytical mass spectrometry

The current major research focus of our laboratory involves the development of fundamental and applied bioanalytical mass spectrometry-based instrumentation and associated measurement strategies for comprehensive and quantitative 'multi-omic' analysis (including transcriptomes, proteomics and lipidomics) and their application toward determining the functional roles of lipids and proteins in the regulation of normal cellular function and the onset and progression of diseases, including cancer.

Ultimately, the results obtained from these studies can provide critical insights toward improving our understanding of disease pathogenesis and may enable the identification of candidate biomarkers for improved disease diagnostic or prognostic monitoring, or novel targets for therapeutic intervention.



An ultra-high resolution / accurate mass spectrometry OrbitrapTM mass analyser for chemical and biomolecular analysis



Advanced mass spectrometry strategies for the comprehensive structural characterisation of lipids.

An early warning monitoring system for illicit drug use.

Professor Mark Rizzacasa

Professor Mark Rizzacasa

- Total chemical synthesis
- Natural products
- Synthetic methods

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My mission is to further the science of organic synthesis by producing rare molecules with novel biological properties and develop new synthetic methods to simplify the production of complex molecules.

Synthesis of alkyl citrate natural products

Our group have been actively pursuing the total synthesis of complex fungal metabolites such as the alkyl citrate family of natural products. These compounds are potent inhibitors of squalene synthase, the enzyme that catalyses the first pathway-specific step in cholesterol biosynthesis. As part of a new research program, we are developing a highly efficient approach to this class of natural products from cyclobutene diesters.

Synthesis of rare biologically active natural products

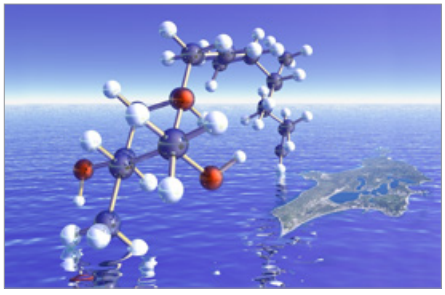
Many biologically active natural products are only isolated in minute amounts, which precludes further investigation into the biological activities of these compounds. We have completed the total synthesis of a number of rare natural products and investigated the modes of action for some of these products.

Development of new hydration catalysis

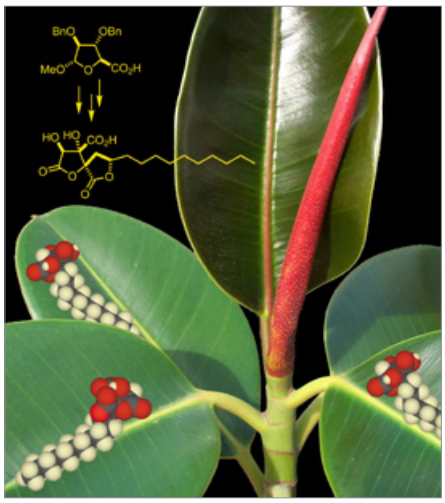
We have recently developed new manganese and cobalt catalysts for Mukaiyama alkene hydration. In addition, efforts have focused on metal octahedral complexes with the goal of effecting this important transformation asymmetric. We have synthesized a number of novel metal complexes that act as efficient catalysts for the Mukaiyama hydration of polar alkenes.

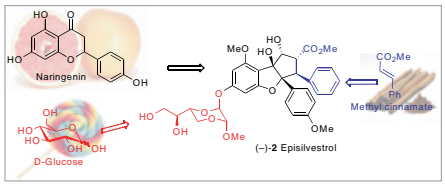
Late-stage oxidation in total synthesis

Late-stage oxidation is utilised in nature for efficient routes to complex, highly functionalised bioactive natural products. Advances in catalysis, genomics and bioengineering can be exploited to furnish enzymes for complex conversions that can closely mimic conditions comparable to those in a living cell. We are currently investigating reactions involving novel catalysts and isolated enzymes to probe the innate reactivity of carbon-hydrogen bonds for key conversions. The ultimate goal of this work is to find shorter and more efficient novel routes to complex molecules to allow for the further study of these compounds.



A molecular model of the marine metabolite rottnestol with Rottnest Island WA, where the compound was first isolated, in the background.





Professor Frances Separovic

Professor Frances Separovic

- Antimicrobial peptides
- Membrane biophysics
- Phospholipid membranes
- Solid-state nuclear magnetic resonance
- Structural biology

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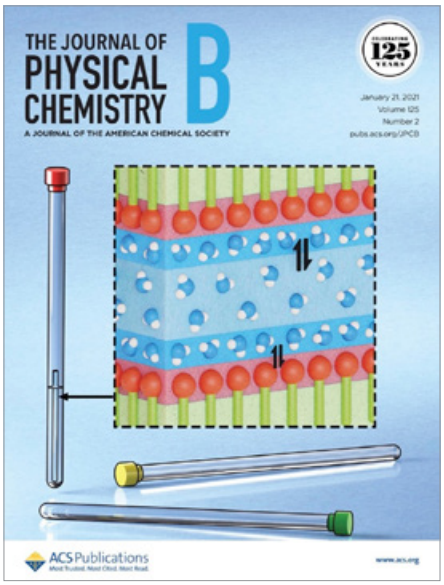
We are trying to determine at an atomic scale how antimicrobial peptides and toxins destroy cell membranes and kill bacteria. The aim is to understand how these molecules function and design more selective peptides that specifically attack pathogens.

NMR and membrane biophysics

Nuclear magnetic resonance (NMR) spectroscopy, complemented by a range of biophysical techniques, is being used to determine the mechanism of action of membrane polypeptides. Our primary goal is to do this for membrane components in model membrane systems as well as live cells. We have determined the 3D structure of two peptides - the antibiotic gramicidin A and the bee toxin melittin - in phospholipid membranes using solid-state NMR methods that are now being extended to membrane proteins.

Our current focus is on the structure and interactions of amyloid peptides from Alzheimer's disease, pore-forming toxins and antibiotic peptides in model biological membranes. Together with other multidisciplinary research groups, we investigate biological macromolecules, geopolymers and ionic liquids for pharmaceutical and industrial applications.

Cover art from Chemical Society Reviews based on our article, Chemically modified and conjugated antimicrobial peptides against superbugs, by Li et al. (2021) Chem. Soc. Rev. 50, 4932-4973.



Cover art from The Journal of Physical Chemistry B based on our article, Chemical exchange of hydroxyl groups in lipidic cubic phases characterised by NMR, by Meikle et al. (2021) J. Phys. Chem. B 125, 571-580.

Professor Trevor Smith

Professor Trevor Smith

- Ultrafast laser spectroscopy
- Microspectroscopy
- Kinetics

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We aim to identify the species formed following the absorption of light in advanced materials, track their dynamics, and map their heterogeneity. This will lead to the more efficient harnessing of light energy in solar energy conversion, better probes of biological systems, and new optical devices and sensors.

Time-resolved microspectroscopy of advanced materials

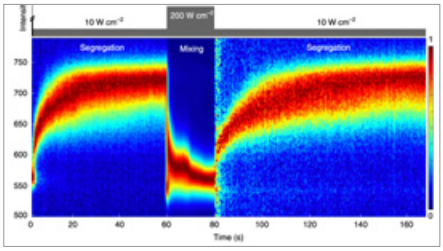
We use advanced optical spectroscopy methods, and resolve the signal in time to investigate changes driven by the interaction between light and new materials. Light-induced processes such as energy or electron transfer can occur on timescales spanning many orders of magnitude (from femtoseconds to milliseconds), and the dynamics of these processes are crucial to the way molecules behave following the absorption of light. Increasingly, it is important to map photomolecular processes and their dynamics on microscopic scales. This requires the development of advanced time-resolved and optical microscopy techniques, and coupling these two approaches together. Such measurements are of direct relevance to light harvesting materials, optical switches, biological and botanical systems and even forensics.

Polarised fluorescence

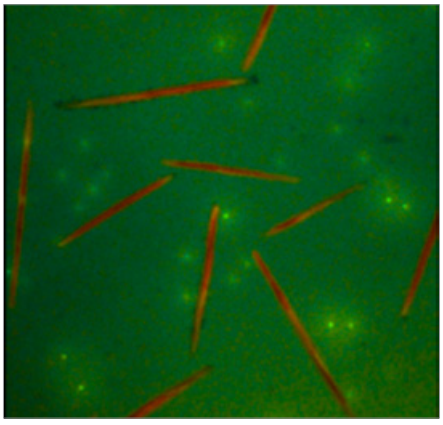
We use polarised light to probe the emission from fluorescent molecules, which can become depolarised due to processes including molecular motion and energy transfer. By monitoring the rate and extent of emission depolarisation we can extract information about the local environment of the fluorophore and its dynamics. These measurements can be applied microscopically to map these processes spatially.

Ultrafast transient infrared spectroscopy

Infrared spectroscopy can be used to identify chemical species through the vibrational modes of specific bonds in molecules. By combining ultrafast laser excitation with infrared spectroscopy techniques, the identity of excited state species and their dynamics can be determined on timescales of femtoseconds to microseconds. This provides information on the contribution various chemical groups make in the excited-state behaviour of molecules. We are developing such techniques to probe the species involved in light harvesting, particularly to identify the short-lived species involved in bimolecular processes such as singlet fission and upconversion, which are approaches to increase the efficiency of solar energy collection.



Light-induced reversal of halide ion segregation in perovskites.



Time-resolved fluorescence image of conjugated polymer (green) and electron acceptor rich (orange) regions in a blended film.

Dr Jegadesan Subbiah

Dr Jegadesan Subbiah

- Organic and perovskite solar cell
- Interface engineering of organic semiconductor
- Device physics of organic photovoltaics
- Synthesis of nanomaterials

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My group focus on the development of high-performance organic and perovskite solar cells through device optimisation, morphology control of the photoactive layer, and interface engineering of the photovoltaic device. We are also interested in developing renewable energy conversion and storage devices for a sustainable clean energy future.

High-performance organic/perovskite solar cells

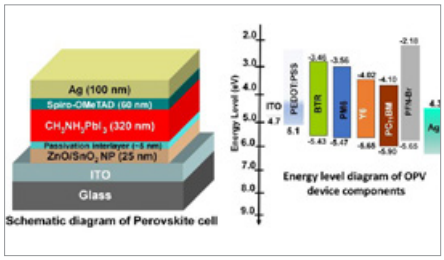
Organic/Perovskite photovoltaics are considered a promising solar energy conversion technology due to their potential to provide large-area solution-processable, lightweight, low-cost and flexible devices. In my lab, we explore the development of solution-processed energy materials, new device architectures, and developing new processing methods for high-performance photovoltaic devices.

Our current research is mainly on the technology development and process optimisation towards the fabrication of efficient organic and perovskite photovoltaic devices, with a prime focus on translational device fabrication from lab-scale devices to large-area printable devices.

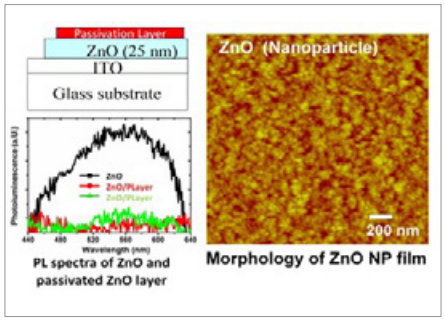
Interface engineering and photophysics of organic photovoltaics

Charge transport, extraction, and collection play important roles in the fabrication of efficient organic solar cells, and interface engineering is one of the key factors in realizing high-performance devices. A good interface can effectively improve the contact between the active layer and the electrode, promote the formation of an Ohmic contact, adjust the electrode work function, reduce bimolecular recombination, increase the charge extraction and enhance the long-term stability of the device.

In our lab, we adopt various approaches, including an ultra-thin layer of polymer materials, doped small molecule materials, and nanostructured metal oxide interlayer to improve device performance and stability.



Device geometry of perovskite solar cell and Energy level diagram of OPV device components.



PL spectra and morphology of zinc oxide nanoparticle interlayer.

Associate Professor Georgina Such

Associate Professor Georgina Such

- Polymers
- Stimuli-responsive systems
- Nanoparticles
- Drug delivery
- Cell interactions

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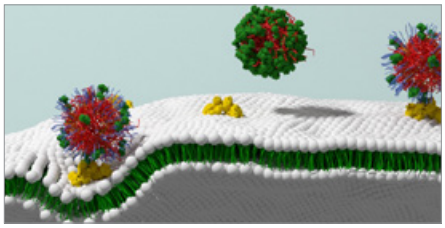
The aim of my work is to design materials that mimic the precise stimuli-responsive capabilities inherent within biological materials such as enzymes in order to develop simple and elegant solutions to complex societal problems.



Development of stimuli-responsive polymer nanoparticles with enhanced versatility and function

The Functional Materials group is interested in the development of new techniques to synthesis nanoparticles that can respond intelligently to changes in their environment, for example variation in pH, redox conditions, temperature or light. We combine polymers with different building blocks such as biological or inorganic materials to maximise the versatility of our materials. We have extensive experience in the development of stimuli-responsive nanoparticles for a diverse range of applications from drug delivery systems through to industrial coatings.

Understanding how nanoparticle structure impacts biological interactions

Nanoparticle delivery systems have potential to improve the treatment of many diseases by targeting drugs to a specific treatment site. However, there are still many challenges with achieving efficient nanoparticle delivery. In our work, we utilise expertise in polymer science and nanotechnology to design libraries of nanoparticles with tailored characteristics, and we use these materials to probe understanding of the impact of nanoparticle structure on biological properties such as cell association, uptake and drug delivery. This work has important implications for improving the design of polymer nanoparticles.

Professor Uta Wille

Professor Uta Wille

- Physical organic chemistry
- Synthetic organic chemistry
- Environmental chemistry
- Computational chemistry

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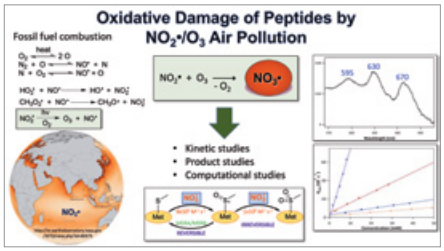
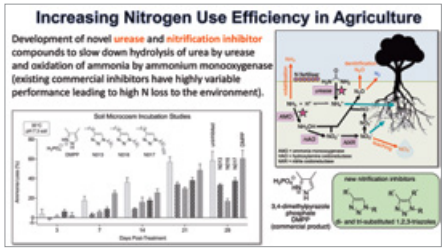
I am passionate about our environment. Chemistry is a highly valuable tool to gain better understanding of the adverse effects of air pollution and to increase the environmental friendliness of agriculture by developing better inhibitor compounds. We are using a wide array of scientific methods for our research, ranging from synthetic chemistry, mechanistic studies, soil incubations and microbiological experiments, which provides students with a variety of skills to prepare them for their future in the workforce.



Oxidative damage of peptides by nitrogen dioxide/ ozone air pollution.



Increasing nitrogen use efficiency in agriculture.

Air pollution and respiratory health

Nitrogen dioxide and ozone are noxious gaseous pollutants produced through the burning of fossil fuels. We know that these gases are bad for us, but we do not exactly understand what happens when we are inhaling these pollutants, which is the primary pathway for exposure. We are using in vitro model systems (in other words: test tube experiments with small representatives of important biomolecules) to gain fundamental understanding of how nitrogen dioxide/ozone air pollution damages biological molecules that are lining the respiratory tract, in particular peptides. Through a combination of product, kinetic and computational studies, we are able to identify hot spots for oxidative damage in peptides and have shown that the environment of an amino acid residue in a peptide has a strong impact on its susceptibility to oxidation.

Increasing nitrogen use efficiency in agriculture

Providing food for a constantly increasing world population has become a major challenge for society. To ensure adequate food resources by 2050, it is expected that the annual crop production needs to increase by almost 40%. A common practice to maximise both soil fertility and crop yield in agricultural systems is through the use of nitrogen (N) fertilisers. Unfortunately, plants assimilate only a fraction of the applied fertiliser N; globally the nitrogen use efficiencies (NUEs) have remained at around 50% since the 1980s. Important pathways responsible for the undesired loss of nitrogen from the plant/soil system include leaching of nitrate, which causes damaging eutrophication of surface waters and groundwater pollution as well as denitrification and emission of the potent greenhouse gas nitrous oxide into the atmosphere. To reduce the mismatch between N supply and plant uptake, fertilisers are commonly amended with inhibitor compounds that slow down microbiological transformation processes, in particular, hydrolysis of urea to ammonia by the enzyme urease (urease inhibitors) and oxidation of ammonia to nitrate by ammonia monooxygenase (nitrification inhibitor). As the existing commercial inhibitor products are characterised by highly variable performance, we are developing new compounds to increase NUEs in Australian soils.

Professor Spencer Williams

Professor Spencer Williams

- Carbohydrates
- Enzymes
- Chemical biology
- Medicinal chemistry
- Glycoimmunology

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We design and synthesize biologically active molecules that we use to probe and study biological systems. We collaborate heartily and widely to maximise the impact of our research. We believe that new discoveries at the interface of chemistry and biology will improve human health and place our industrial and agricultural systems on a more sustainable path.

Glycolipid immunology

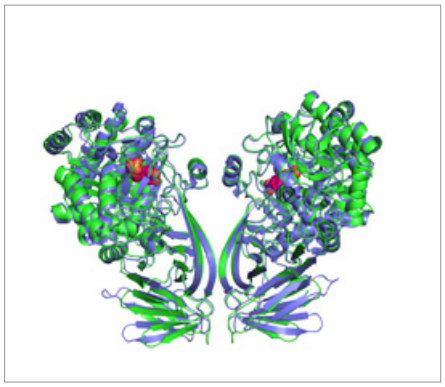
We synthesize biologically active glycolipids that are difficult or impossible to obtain from nature, and once we have established strategies for their synthesis we explore structure-activity relationships. We are interested in how the immune system can recognise foreign glycolipids from pathogens and commensals and work with collaborators to explore their effect on the immune system.

Chemistry and biology of carbohydrate-active enzymes

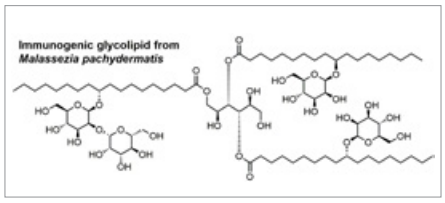
We are interested in understanding the mechanism of enzymes that process carbohydrates. Using organic chemistry, we make substrates and inhibitors used in kinetic and structural studies to illuminate how enzymes work at the molecular level. We collaborate with structural biologists, computational chemists and biologists who use our substrates and inhibitors to dissect enzyme mechanism.

Medicinal chemistry

The ultimate biologically active molecules are drugs. We are interested in developing drugs to treat several human diseases, including lung and kidney fibrosis, cardiovascular disease and sterile inflammation. Projects in this area involve structural optimisation to enhance potency or improve pharmacokinetic and metabolic liabilities. We collaborate with pharmacologists, modellers and biologists with animal models of disease.



3D structure of bacterial sulfoquinovosidases revealed how it binds substrate and perform catalysis.



Total synthesis of an exotic fungal glycolipid from Malassezia pachydermatis.

Associate Professor Wallace Wong

Associate Professor Wallace Wong

- Dyes
- Organic semiconducting materials
- Exciton science
- Light harvesting
- Chemical sensing

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The vision for my research is to address fundamental scientific problems in the development of materials for emerging technologies. These technologies can be applied to problems in energy and the environment as well as biology and medicine. The main fundamental scientific problem we regularly tackle is multi-scale materials design and synthesis. With the current knowledge, it is possible to design and produce new compounds with desired molecular properties with reasonable precision.

However, given the molecular structure, the prediction of bulk properties and functionality of the materials in devices remains a huge challenge. This gap in knowledge in material science is due to the fact that bulk properties are derived from not only the molecular properties but also from intermolecular association and ultimately macromolecular arrangement in the nanometre scale.

Organic electronics

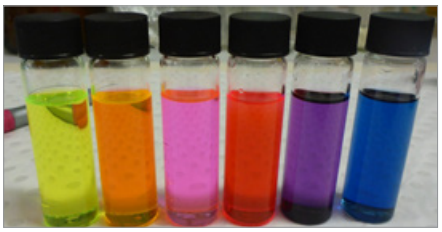
The emergence of organic electronics is transforming current electronic technologies that will lead to light weight flexible devices such as foldable displays, building-integrated lighting and low-cost solar cells. The greatest improvements in efficiency and durability of devices will be achieved through precise control of material structure from molecular to bulk scales. We are addressing this problem by designing smart materials that can self-organise and enhance the properties required for specific applications.

Light harvesting

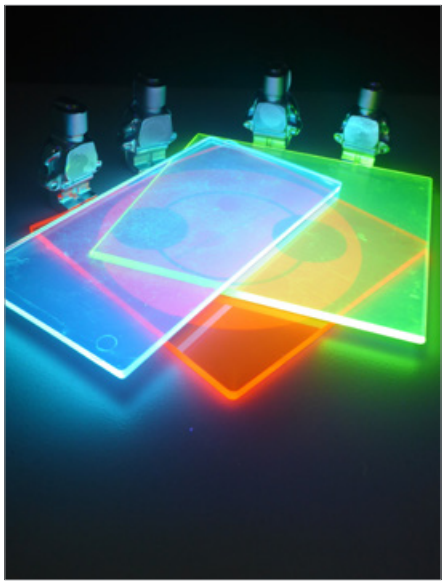
Efficiently harvesting the full solar spectrum and integrating solar cells in urban areas, ie building-integrated photovoltaics are both areas of interest in our group. We design and study triplet fusion and singlet fission materials to refine the solar spectrum. This compression of the solar spectrum enhances solar cell performance leading to cost reduction of solar energy. We work on highly fluorescent materials for use in luminescent solar concentrators, a type of solar collector that can be easily integrated into architectural structures and other urban objects.

Biological imaging

The development of advanced fluorescence microscopy techniques and fluorescent agents has greatly increased the information obtained from imaging biological samples. Cleverly designed and carefully chosen organic fluorophores can target specific cells, organelles, membrane receptors and/or protein-active sites. We have expertise in the synthesis and characterisation of multi-functional stimuli-responsive fluorescent dyes. We use these dyes to track proteostasis and other biological processes.



Beautiful colours as a result of highly tunable organic dye structures.



Fluorescent sheets used in luminescent solar concentrators to harvest solar energy.

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