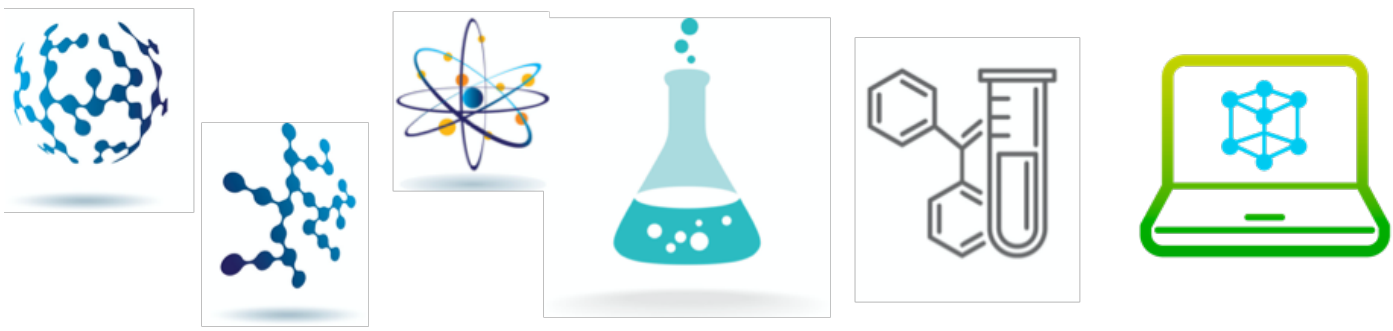
THE UNIVERSITY OF
NEWCASTLE
AUSTRALIA

DISCIPLINE OF CHEMISTRY

HONOURS AND UNDERGRADUATE RESEARCH PROJECTS

2024



Undergraduate Research in the Discipline of Chemistry

School of Environmental and Life Sciences

There are a number of strong research themes in the discipline of chemistry in areas such as:

- Functional materials for health, environment and energy
- Medicinal Chemistry
- Computational chemistry
- Molecular organic synthesis
- Colloids, interfaces and soft matter

We encourage undergraduates to get involved in research throughout their degree. By doing so you will learn and develop skills in searching, selecting and retrieving information from scientific sources, skills in project management, experimental research skills as well as skills in presenting scientific information in a clear and concise manner, both orally and in writing. These will provide you with a strong foundation for your future career, whether it be in the industrial, commercial or academic sector.

There are three main ways to get involved in research:

a) ***Summer research project:*** Short paid undergraduate research projects over summer. Scholarships are advertised each year

b) ***SCIE3500:*** Complete a research project under the supervision of an academic staff member as an elective 10 credit point subject. The course is open to third year students who have successfully completed at least 140 units and have a cumulative GPA of at least 5.0 and is offered in both semesters. Course outline link here.

c) ***Honours research project:*** A full-year research project after completion of the Bachelor of Science or another cognate degree. A minimum GPA of 5.0 is required for entry into honours. Program handbook link here.

This booklet contains a list of undergraduate research projects currently available in the discipline. Academics are listed in alphabetical order. In all cases you should discuss potential projects with prospective supervisors before trying to enrol or apply.

Dr Jennifer Baker

Unavailable S1 2024

Computer-Aided Drug Design and Synthesis

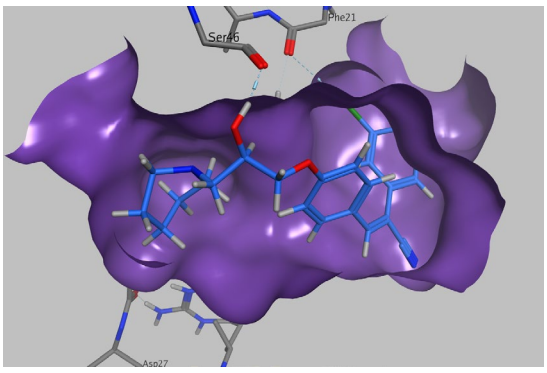
Website: https://www.newcastle.edu.au/profile/jennifer-r-baker
Contact email: jennifer.r.baker@newcastle.edu.au

Computer-aided drug design is a method of drug design that involves one of two broad methods: structure-based drug design, and ligand-based drug design. The most common, and the main method Jennifer utilises, is structure-based. This is where the 3D structure of the desired biological target is known, either with an experimentally determined crystal, NMR, or cryo-electron microscopy structure, or an experimentally derived homology model. Utilising this knowledge of the biological target, new small molecules can be designed that maximise binding affinity with the biological target, resulting in only the synthesis and biological testing of the best and most promising small molecules. The majority of Jennifer and her team's work is on the design and synthesis of KDM4 analogues (described below), but she is also interested in the design and synthesis of AhR ligands.

a) Computational design, histone lysine demethylase protein 4 (KDM4): The KDM4 protein has a key role in postranslational histone modifications, primarily methylation, which control subsequent cell proliferation and transcriptional control. Disruption of these modifications via competitive binding of a small molecule into the active site of KDM4 results in disruption of cancer cell proliferation. Utilising the solved crystal structure of KDM4, molecular modelling methods such as receptor-ligand docking and fragment-based drug design can be exploited to design small molecules that have improved affinity within the active site of the protein. Using Molecular Operating Environment (MOE), and AutoDock Vina for receptor-ligand docking runs, and MOE for subsequent molecular dynamics studies, you will design new small molecules that will subsequently be synthesised and sent for biological analysis in a KDM4 AlphaScreen with collaborators at the University of Sydney.

b) Synthesis of inhibitors of KDM4: With knowledge of the most promising inhibitors of the KDM4 catalytic site, as part of this project you will synthesise a select, focused number of small molecules using a range of organic chemistry methods. A selection of different small molecule libraries are available to be optimised for KDM4 inhibitory activity, with synthetic design primarily led by the computational examination of the binding site of KDM4; as well as structure-activity relationship studies of previously synthesised and tested small molecules. Organic synthesis, purification and characterisation will be conducted in the research labs in Newcastle, with subsequent biological testing conducted by our collaborators at the University of Sydney.

c) Computational design, Arylhydrocarbon Receptor (AhR): The Arylhydrocarbon Receptor is a nuclear translocator that has been shown to be upregulated in certain breast cancers. Methods of exploiting the pathway of this protein include either 'hijacking' it to gain access to the nucleus of cancer cells or inhibiting it via binding with its catalytic site to prevent its action in cell proliferation. Using a homology model prepared in conjunction with A/Prof Stefan Paula from California State University, you will use methods such as receptor-ligand docking and fragment-based drug design to design new small molecules that fit well within the binding site. As the crystal structure has not been experimentally determined, you may also use



ligand-based drug design in this project: this is the method where structures of known active AhR ligands are used to aid the design of new molecules with good affinity.

d) Synthesis of inhibitors and activators of AhR: Building on from previous study of AhR ligands, as well as examination of the binding site, you will design and synthesise a range of ligands with either targeted inhibitor or activator roles, with differing human disease targets. Our group has been studying the AhR for the potential future treatment of breast cancer for a number of years, with a broad range of previously collected structure-activity data available to aid in the design of new small molecules. Synthesis, purification, and characterisation will be conducted in Newcastle, with biological analysis conducted by our collaborators at the Calvary Mater Hospital in Waratah.

Dr Robert Chapman

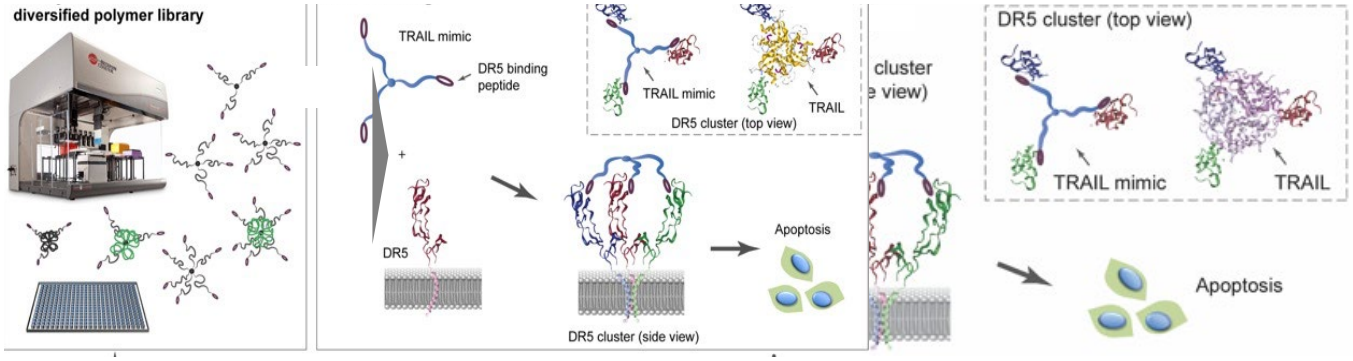
Polymer therapeutics and protein mimics

My group uses ***high throughput polymerisation techniques*** to design polymers that will fold like proteins do to make better therapeutics, and to design polymers that will bind to and stabilise proteins and antibodies

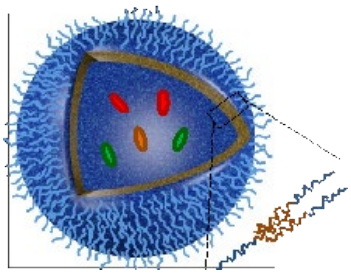
Website: www.chapmangroup.org
Contact email: robert.chapman@newcastle.edu.au

My group's research centres on our ability to polymerise complex polymers in high throughput using a robot, which allows us to screen how the polymer's structure affects its function.

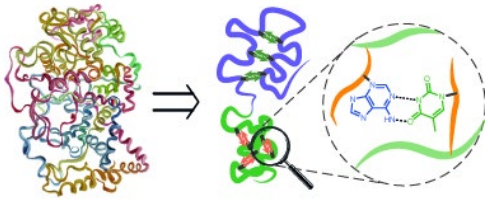
a) Macromolecular therapeutics by high throughput synthesis *(with Dr Thomas Fallon).* Since its discovery in the late 1990s, the TRAIL protein (tumour necrosis factor related apoptosis inducing ligand; also known as Apo2L), has been widely pursued as a highly selective and potent chemotherapeutic across a wide variety of cancers. Yet, despite a massive research investment from both academia and industry, all variants of the TRAIL protein have failed to show efficacy in the clinic to date due to the protein's poor stability and bioavailability. We are using a high throughput polymerisation method established in our lab to make synthetic mimics of TRAIL that can replicate it's biological activity but which have vastly improved pharmacokinetics (circulation times of up to 50 h).[1-2] The project involves a mixture of synthetic organic chemistry, polymer chemistry, and *in-vitro* cell assays.

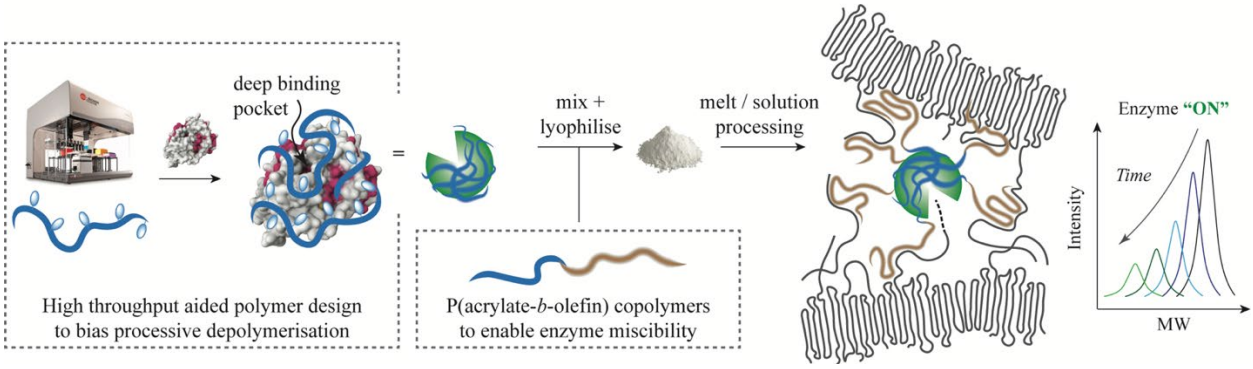


b) Protecting the nitrogenase enzyme to make a nitrogen battery *(with CSIRO Canberra).* We are interested in using a natural enzyme called *nitrogenase* for the electrochemical conversion nitrogen to ammonia, for energy storage applications. *Nitrogenase* is extremely efficient at driving this reaction, but its use is hampered by its sensitive to oxygen. This project will focus on developing methods to stabilise the enzyme by co-encapsulating it in a polymersome with another enzyme called *glucose oxidase*, which is able to consume oxygen. This should stabilise nitrogenase, and enable it to be used in regular oxygenated solutions. The project forms part of a larger project with CSIRO Canberra. Our collaborators have developed excellent and robust techniques for preparing and isolating the enzyme from bacterial cultures, and will supply the enzyme for our work.



c) Depolymerisation of plastic waste using polymer-coated enzymes *(with Prof Erica Wanless & Prof Dominik Konkowlewicz).* This project aims to design polymer coatings for enzymes that will enable them to be embedded into polyethylene, and later activated to in a compost heap to decompose the plastic to small molecules. Enzymes are normally very difficult to disperse in polyethylene, but we have recently developed a range of chemistries to prepare polyacrylate-polyethylene block copolymers that should enable this. By using high throughput polymer synthesis and screening techniques that we have already developed,[3] this project will design polyacrylates that bind strongly to a polyethylene active enzyme called *manganese peroxidase*, and then synthesise polyacrylate-polyethylene block copolymers from these to enable encapsulation of the enzyme in a bulk matrix of polyethylene.





d) Sequence defined oligomers by decarboylative click reactions *(with Dr Thomas Fallon).* Most large biological molecules (proteins, RNA, DNA) are sequence defined polymers – the exact ordering of monomer units is specifically defined. There are relatively few ways to replicate this synthetically. We can make relatively long peptides by sequential amide bond formation but this must be done on a solid support to enable efficient removal of the protecting groups between each coupling reaction. A solution phase synthesis, that doesn't result in any byproducts would enable synthesis of complex oligomers at scale. By extensive screening we have discovered reaction conditions for the azide-alkyne click reaction at which the certain alkyne protecting groups (such as -CO_2H) are stable. The protecting group can then be removed with either heat or light. This project will develop these protocols into an efficient solution phase synthesis of sequence defined polymers.

Selected References:

1. Li, Z.; Kosuri, S.; Foster, H.; Cohen, J.; Jumeaux, C.; Stevens, M.; Chapman, R.; Gormley, A.; ***J. Am. Chem. Soc.*** 2019, 141 (50), 19823–19830.
2. Li, Z; Han, Z.; Stenzel, MH; Chapman R.; ***Nano Lett.*** 2022, *22*, 2660–2666.
3. Mustafa, A. Z.; Kent, B.; Chapman, R.; Stenzel, MH; ***Polym. Chem.*** 2022, 13 (43), 6108–6113.

Dr Sam (Xianjue) Chen

Materials Chemistry, Carbon Materials

My research group are working on '**artificial materials**', particularly new carbon-based materials, through developing new synthesis strategies and applications of materials.

Website: https://www.samchenlab.com
Contact email: sam.chem@newcastle.edu.au

---

a) Diamane. Single-layer diamond structure ('diamane') has emerged as a new 2D form of carbon which was first predicted theoretically followed by recent experimental realisation. In collaboration with Prof Marc Dubois (UCA), my team reported the experimental preparation of fluorinated diamane ('F-diamane') from graphite flakes (Carbon, 2021, 175, 124; Appl. Surf. Sci., 2022, 152534). These are the first reports in which diamane-like materials are prepared using a 'top-down' chemical route.

b) Graphene. We have worked with Prof Rodney Ruoff's group (UNIST, CMCM) on the growth, transfer, and folding/stacking of graphene films, including (i) growth of centimetre-wide, AB-stacked bi-layer and ABA-stacked tri-layer graphene films (Nature Nanotechnol. 2020, 15, 289); (ii) non-destructive delamination for transferring CVD graphene (Chem. Mater. 2017, 29, 4546); (iii) folding of single-crystal graphene with defined stacking orders (Nano Lett. 2017, 17, 1467); (iv) layer-by-layer assembly of graphene into macroscopic films (Adv. Mater. 2019, 31, 1909039).

c) Fullerene. Fullerenes, particularly C_{60}, are the only forms of carbon nanomaterials to date that can be made with precisely controlled molecular structures. Our latest research efforts include using fullerenes as molecular building blocks to construct new 'artificial' carbon materials, such as C_{60}-graphene hybrid structures, self-standing C_{60} networks, etc.

d) Chemistry in confined space. Graphene and carbon nanotubes can be used as 2D and 1D 'nano-reactors' for chemical reactions. Such dimensional confinement can lead to new reactions and phenomena that are less explored in the field of chemistry.

These projects are based on experiments in chemistry laboratory, which require the use of advanced microscopic and spectroscopic techniques at the Central Analytical Facilities for material analysis, including transmission electron microscopy (TEM), scanning electron microscopy (SEM), atomic force microscopy (AFM), X-ray diffraction (XRD), Raman spectroscopy, X-ray photoelectron spectroscopy (XPS). Depending on the nature of research project, the candidate will be supported for training and accessing these instruments.

I'm open to other project ideas. Please feel free to send me an email (sam.chen@newcastle.edu.au) or simply drop by my office in C216 Chemistry Building, Callaghan Campus.

Prof Scott Donne

Electrochemistry and energy storage materials

Website: https://www.newcastle.edu.au/profile/scott-donne
Contact email: scott.donne@newcastle.edu.au

My main research interests lie in the general area of electrochemistry, particularly on energy storage materials such as batteries, supercapacitors and fuel cells. In this area we focus on the preparation of new materials, and then evaluate their behaviour and performance under a variety of conditions. While this represents research in only a relatively focussed part of electrochemistry, I do also have significant experience in electrodeposition, the application of various electroanalytical methods, as well as in the study of corrosion. At present I also have a number of ongoing projects dealing with industrial chemistry.

a) Advanced Supercapacitors: Modern electronic devices (e.g., consumer electronics and electric/hybrid vehicles) place considerable demands on their respective power sources, to the point where device efficiency is compromised. The inclusion of a supercapacitor has the potential to improve the specific power density and also cycle efficiency of all types of power source. We have recently made considerable advances in improving supercapacitor performance (e.g., 800 F/g for existing systems compared to >2000 F/g in our advanced materials). Projects in this area will be focus on both understanding the origin of this improved performance, as well as implementing these materials into prototype supercapacitors. This work is funded by CSIRO Division of Energy Technology and CAP-XX, and is also in collaboration with the Ecole Polytechnique de la Universitie de Nantes and National Taiwan University.

b) Catalysts for Fuel Cells: Energy can be stored in many chemical forms, and hence used in many different ways. One way is in a fuel cell, of which there are numerous varieties. The cathodic reaction in all though involves reduction of O_2 to H_2O on the surface of a suitable catalyst. This is currently the limiting performance feature of all fuel cell technologies because of its slow reaction kinetics. This focus of projects in this area is to examine the factors that cause slow O_2 reduction kinetics, and to then address these limitations with novel solutions. One particularly important aspect is to examine the role that adsorption plays in determining O_2 reduction kinetics. This work is in collaboration with the Massachusetts Institute of Technology.

c) Corrosion Phenomena in Electrode Materials: Corrosion is an electrochemical phenomenon that can have a devastating effect on all forms of infrastructure if it is not properly monitored and controlled. Projects in this area are focussed on understanding the corrosion phenomena that metals such as titanium and copper undergo, and then developing strategies to minimize their corrosion. Titanium, for example is used as the anode substrate in many modern high volume electrolysis processes, yet it is subject to corrosion and passivation which effectively destroys its performance. Similarly, copper is used as an earthing electrode in modern power infrastructure, in which case its corrosion and failure lessens the safety of such a network. Support for these projects comes from Energy Australia.

d) High Performance Battery Systems: The backbone of energy storage in modern society is the battery. Of course many systems are commercially available, each having been developed to power a specific type of electronic device. The importance and extent of efficient energy storage will increase in the future due to the required move away from fossil fuel powered energy. Projects in

this area will focus on the development of advanced materials, and improving our fundamental understanding of the charge storage mechanisms various materials possess. Funding in this area comes from the CSIRO Division of Energy Technology (Li-ion systems), Duracell (advanced MnO_2), Pure Energy Battery Systems (rechargeable MnO_2), and Litronik Batterietechnologie (battery systems for implantable pacemakers).

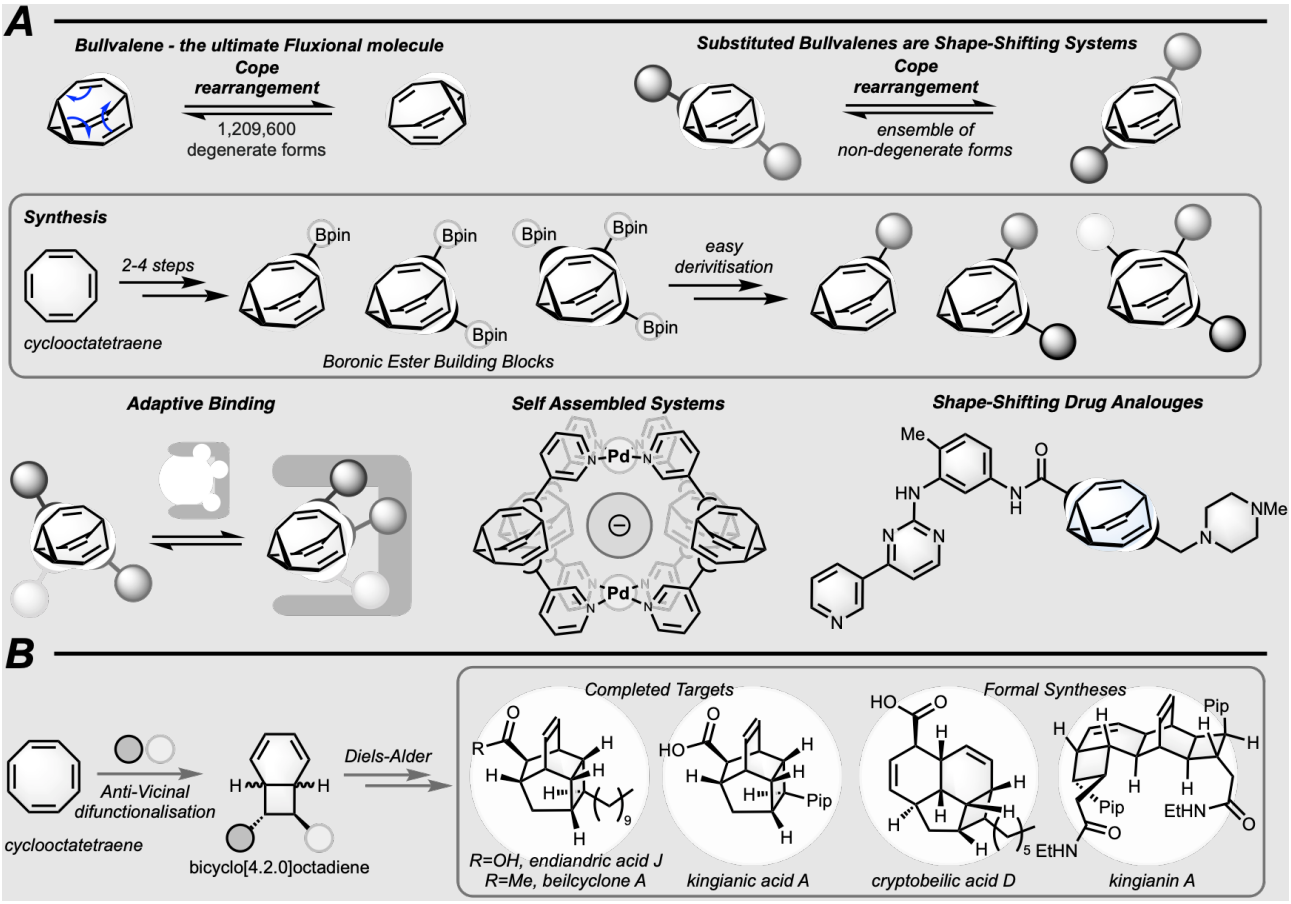
e) Hydrogen Production: Hydrogen has been variously described as the perfect fuel. It is abundant, chemically non- toxic, and it burns to produce non-toxic species. However, its main limitation to commercial uptake is its synthesis, since it requires more energy to produce hydrogen than what is returned upon its combustion. Projects in this area revolve around the use of the Hybrid Sulfur (HyS) Cycle for the large scale production of hydrogen. Using renewable energy inputs water can be split into its components through the use of a sulphur-based intermediate. Part of the HyS cycle involves an electrolysis step (SO_2 oxidation to H_2SO_4), the efficiency of which is a significant limitation to the overall process. Therefore, our focus will be on developing an understanding of the oxidation mechanism, and developing new catalysts to facilitate its improvement. This work is in collaboration with the CSIRO Division of Energy technology.

Dr Thomas Fallon

Shape-Shifting Molecules and Natural Products Synthesis

Website: www.fallon-lab.org
Contact email: thomas.fallon@newcastle.edu.au

Our group develops new methods and strategies in synthetic organic chemistry to make structurally complex molecules. In one theme of research we study the chemistry of shape-shifting molecules (Figure A). Bullvalene is an extraordinary structure that spontaneously exists in over a million degenerate forms and has no permanent carbon-carbon bonds. This unique molecular behaviour opens up many potential applications. We have developed easy methods to make substituted bullvalenes which exist as ensembles of shape-shifting isomers. Projects in this area will seek to explore the applications of shape-shifters in adaptive binding, self-assembled systems, and drug analogues. We are also interested in using shape-shifting molecules in new catalysts, molecular machines, and materials chemistry.



Another theme of research in the group is the synthesis of structurally complex natural products (Figure B). The *endiandric acids* and related natural products have all been isolated from the *Lauraceae* family of plants endemic across northern Australia and Southeast Asia and have a wide

range of potent biological properties reported. They also share a spectacular biosynthetic origin – a pericyclic reaction cascade. While most laboratory researchers have sought to intercept this cascade reaction, our group has developed a short cut that allows us to make these targets in just a few reaction steps. We are now able to make a wide range of these molecules, as well as analogues, which will enable their further biological studies. Projects in this area will seek to develop medicinal chemistry libraries related to the endiandric acids, as well as targeting the synthesis of other complex natural products.

A/Prof Clovia Holdsworth

Unavailable in 2024

Molecularly imprinted polymers

Website: https://www.newcastle.edu.au/profile/clovia-holdsworth
Contact email: clovia.holdsworth@newcastle.edu.au

I trained as a polymer chemist with considerable experience and knowledge in radical polymer synthesis with focus on polymer functionalisation and the use of these synthetic methodologies for the synthesis of specialised polymers for various applications. One of my research interests is molecular imprinted polymers (MIPs), their utility as extractants and sensing materials and optimisation of synthesis and performance.

a.) Molecularly Imprinted Polymers (MIPs): Molecular imprinting is an effective method of imparting highly specific and selective recognition sites in synthetic polymers. First, a molecule of interest (target) is used as the template and allowed to pre-associate with polymerisable (a molecule with a double bond) molecules (*in situ* imprinting) called the functional monomers. The degree of association between the monomer and the template (T) depends on their functionalities but mostly based on simple molecular interactions such as hydrogen-bonding. Secondly, the association between the template and monomer can be fixed in place by polymerisation in the presence of a huge amount non-interacting monomer (e.g. crosslinker), which can impart the robustness required for the polymer. Thirdly, the template is extracted from the monolithic or particulate polymer to leave behind a cavity containing binding sites that are oriented to compliment the functional groups of the template molecule and capable of rebinding the target. Molecular imprinting can also be achieved by *post*-polymerisation imprinting on a pre-prepared polymer, a technique that is very useful for the preparation of 2-D MIP films or beads.

i) *Preparation of MIP Nanofibres:* This project will examine the feasibility of preparing molecularly imprinted polymeric nanofibres by electrospinning. Briefly, the template will be combined with a linear polymer in solution then electrospun. The resulting MIP nanofibers could be useful as specific filters.

ii) *Development of MIPs for Aldehydes and Ketones:* *This* is a novel project that will tackle imprinting of aldehydes and ketones by utilising their characteristic reaction with hydrazines forming hydrazones. Work will entail literature review, design of polymerisable hydrazines/hydrazones and synthesis of MIPs. Extraction will depend on the reversibility of the reaction hence it is also necessary to study the kinetics of the formation and hydrolysis of hydrazones. Potential application of this MIPs is in fragrance industry.

iii) *Towards the development of a MIP-Based Biosensor:* The project will involve the synthesis of MIPs for potential use as a recognition element for an optical biosensor. The MIP will be attached to an optical fiber – the signal transducer. The work will be divided into 2 sub-projects:

- Preparation of MIP: MIPs selective to cyanobacteria compounds, e.g. microcystein-LR, will be prepared using controlled radical polymerization using commercially available atom-transfer radical polymerisation (ATRP) initiator. Template rebinding and selectivity of the MIP will then be evaluated.
- Functionalisation of the optical fiber transducer: This project will involve functionalising the surface of an optical fiber with an atom-transfer radical polymerisation (ATRP) initiator moiety, a test polymerization reaction and possibly MIP attachment.

iv) ***Magnetic MIPs:*** The utility of MIPs as a selective extractant could be enhanced by embedding the polymer with magnetic properties to facilitate the extraction process of an analyte from complex matrices. To create the magnetic MIPs or MMIPs, polymerisation and molecular imprinting is introduced at the surface of magnetic inorganic iron particles. Thus, after analyte capture, the insoluble MMIPs can be simply recovered from the sample matrix by a magnetic separator without the need of filtration or centrifugation. For this proposed project, the aim is to generate MMIPs for 5-fluorouracil (5-FU), a cancer drug, potentially to be used for the capture of residual 5-FU in urine for subsequent quantitative analysis. This project will involve the synthesis of the MMIP particles and evaluating its binding efficiency (target binding capacity, pH effect, stability and strength of binding, selectivity) either by HPLC or NMR.

b) Preparation of Amphiphilic Copolymers for Extraction of Membrane Proteins: The challenge with the studies of membrane proteins is their extraction while preserving their native lipid environment. Styrene maleic acid copolymers (SMA) copolymers have been found to be successful in solubilising and stabilising the membrane proteins by encapsulation by forming SMA-lipid particles (SMALPs). Other polymer variants to form SMALP-like particles have also been studied. While the performance of the SMA copolymers could be optimised by controlling their lengths and composition, their efficacy is limited to near neutral pH. In this project, we will target copolymers with SMA-like properties which will potentially work at low pH. This project will involve synthesis of copolymers by radical polymerisation, molecular weight determination by size-exclusion chromatography and determination of copolymer composition by 1H NMR. Once the copolymers have been characterised and purified, their efficacy in stabilising lipids that contain membrane proteins will be tested.

Prof Adam McCluskey

Medicinal organic chemistry

Website: https://www.newcastle.edu.au/profile/adam-mccluskey
Contact email: adam.mccluskey@newcastle.edu.au

My primary area of research is in the medicinal chemistry / chemical biology space where my main focus is in the development of tool compounds, and drugs, targeting endocytosis. The potential outcomes of our research include (but are not limited to) the development of new synthetic methodologies; the development of new drugs & the development of new tools for dissecting signal transduction pathways.

a) Flow Chemistry / Medicinal Chemistry / Organic Chemistry: Traditional organic synthesis is conducted in a batch manner, i.e. small quantities of materials are mixed and heated for a standard period of time, and the product extracted and purified. Recent advances in flow technologies allow continuous production of novel materials. This technology has been introduced to the medicinal chemistry group at the University; it is currently the best-equipped flow chemistry laboratory in Australia. Reactions are conducted at higher temperatures and pressures, which has the effect of increasing reaction yield and compound purity, largely removing the more tedious aspects of compound purification. Students working in this area will develop new approaches to drugs spanning three research programs: anti-epileptic, anti-cancer and anti-parasitic drugs. This new technology requires subtle optimisation and students will be exposed to cutting edge equipment and ultimately be responsible for the development of new drugs and biological tools to a considerable number of our national and international collaborators.

b) Medicinal Chemistry / Drug Design: Today 1% of the worlds' population suffer from epilepsy, of these 30% fail to respond to existing anti-epileptic drugs. Current anti-epileptic drugs were discovered in the 1960s. We have identified a protein called dynamin as a new ant-epileptic drug target and have advanced compounds that only target epilepsy at seizure onset, a significant advance on existing treatments. This is a major collaborative drug discovery and development effort drawing medicinal chemistry experience at the University of Newcastle (McCluskey), neurobiology and neurochemistry at the Children's Medical Research Institute Westmead Hospital (Prof Phillip Robinson), epilepsy (medical aspects) at the Royal Melbourne Hospital / Melbourne University (Prof Terry O'Brien), and the National Institute of Health (USA). Students working in this area will experience the full drug development cycle through synthesis and biological evaluation of new drugs. You will advance these drugs to the next stage of evaluation and potentially to animal studies in both Melbourne and USA. During the course of your studies you will be trained in the latest technologies associated with drug design and chemical synthesis (see Flow Chemistry above).

Prof Alister Page

Computational chemistry

Website: https://compchem.newcastle.edu.au/
Contact email: alister.page@newcastle.edu.au

The computational materials chemistry group performs fundamental and applied research into self-assembly, complex systems and the structure and properties of material systems, using quantum chemical and molecular dynamics techniques.

a) How do Nanotubes Grow? A carbon nanotube is a sheet of carbon atoms in a chicken wire pattern, rolled up into a cylinder. Although they are only ~1 nanometer in diameter, they can be several millimeters in length, are ~100 times stronger than Kevlar, and can transport ~1000 times as much electricity as copper wires. They can also be both electrically conducting and semiconducting, depending on how the carbon atoms in their structure are arranged. Development of future carbon nanotube-based technologies is currently prevented by our inability to synthesise particular carbon nanotubes selectively. This project will determine how selective carbon nanotube "growth" can be achieved, and will pave the way for the future development of carbon nanotube-based devices.

b) Water Splitting Perovskite Materials: Hydrogen is a superior energy source due to its high energy density and the fact that it produces water as the only chemical product from combustion. One potential method for producing hydrogen is by splitting water, according to the stoichiometric equation $2H_2O_{(l)} \rightarrow 2H_{2(g)} + O_{2(g)}$. Being able split water photocatalytically – i.e. using solar irradiation – is the ultimate goal of hydrogen energy technologies. Recently, a new class of photocatalysts – perovskites – have begun to show significant potential in this area. Perovskites are binary metal oxides with chemical structure ABO_3, where a metal cation A occupies 12-coordinate interstitial sites within octahedral BO_6 units. The aim of this project is to optimise new perovskite materials for photocatalytic water-splitting using computational chemistry.

c) One-Dimensional van der Waals Heterostructures: Atomically-thin 2D materials (graphene, boron nitride, etc.) are the building-blocks of a new and exciting class of functional materials – 2D van der Waals (vdW) heterostructures. 2D vdW heterostructures are formed by 'stacking' multiple atomically-thin 2D materials. Each layer in the stack is held in place via interlayer vdW interactions with its neighbouring layers. 2D vdW heterostructures are the foundation of a new generation of nanoelectronics devices and applications. This project aims to translate the concept of a 2D vdW heterostructure to a single dimension, by understanding the structure and properties *1D vdW heterostructures* - heterostructures composed of inorganic nanotubes held in place via radial vdW interactions – like a nanoscale coaxial cable. The project may also consider how such 1D heterostructures might be formed during chemical vapour deposition synthesis.

d) Origins of Hofmeister Effects: In the late 1800s, Franz Hofmeister discovered that, while some salts would decrease the solubility of egg whites in water, others increased their solubility. This phenomenon is known as the Hofmeister effect. Despite its apparent simplicity, consensus over the origins of the Hofmeister effect still has not been reached. In the century since Hofmeister's discovery, the Hofmeister effect has been observed in a wide range of other dissolved solutes, from DNA, enzymes, surfactants and colloidal suspensions. This project will use molecular simulations to understand the origins of the Hofmeister effect and how dissolved salts influence the solvent structure and properties.

e) Chemical Methods for Cutting Graphene: Graphene is an atomic-scale chicken wire made of a single layer of carbon atoms. Graphene has remarkable properties – it is simultaneously the lightest, strongest and stiffest material known, but still conducts electricity roughly a million times better than copper wires. Current graphene production methods make native graphene “sheets” with widely varying dimensions. This limits the use of graphene in next-generation devices, such as flexible electronics, sensors, fuel cells and drug-delivery systems, because graphene sheet size and shape determine key physical properties. This project will determine new chemical methods that can be used to produce graphene sheets with specific shapes and sizes, towards enabling next generation graphene-based technologies.

Dr Qianqian Shi

Plasmonic nanoparticles and their self-assembly

Contact email: qianqian.shi@monash.edu
or Qianqian.shi.scut@gmail.com

Metallic nanocrystals are important building blocks in the contemporary nanoscience and nanotechnology, which have demonstrated profound implications in the materials chemistry discipline. In particular, gold and silver nanoparticles attract significant attention due to their unique size- and shape-dependent localized surface-plasmon resonances. These nanoparticles, also referred to as 'artificial atoms,' are nanoscale elements that contribute to the creation of an 'artificial periodic table.' They can be used to construct diverse nanoassemblies for novel applications in electronics, photonics, photovoltaics, medical diagnostics, and therapeutics.[1] My primary research focuses on the design and assembly of novel plasmonic nanocrystals with specific functions in photocatalysis, plasmonics and sensing applications. By engineering the materials design including building blocks synthesis, surface functionalization, and bottom-up self-assembly, my group aims to harness the programmable plasmonic properties and soft conductive properties of plasmonic nanocrystals for broad applications in the design of artificial leaves, flexible plasmonic sensors and flexible plasmonic electronics.

a) Flexible plasmonic artificial leaves: This project aims to design and fabricate soft, ultrathin, and large-area 2D plasmonic photocatalysts with natural leaf-like attributes for solar-to-chemical energy conversions. Traditional photocatalysts are colloidal based or supported on rigid and thick substrates. It is challenging to integrate them into soft leave-like devices and achieve leaf-like structure/functions due to their intrinsic mechanical mismatch in Young's moduli. This project directly addresses this challenge by using self-assembly fabrication technologies to fabricate 2D plasmonic nanoassemblies and further constructing soft artificial leaves for a continuous solar-to-chemical conversion.

b) Flexible plasmonic bio-chemical sensing: Plasmonic nanomaterials have been widely used as surface enhanced Raman scattering (SERS) substrate for bio-chemical sensing because of their ultrahigh detection sensitivity and high specificity. However, traditional SERS substrates are typically rigid and it is challenge to provide a seamless contact with the soft and elastic biointerfaces such as epidermis for bio-chemical sensing. This project can bridges this gap by design a flexible composite made from ultrathin and soft 2D SERS-active plasmonic metasurface and a flexible porous polymer. By extracting analytes such as sweat from the body using the porous polymer, the wearable plasmonic biosensor will provide fingerprint detection of trace-amounts drugs inside the body under different deformation states.

c) Flexible plasmonic stimuli responsive sensors: This project aims to design and fabricate soft and ultrathin 2D plasmonic assemblies with high sensitivity towards environmental stimuli. Plasmonic nanomaterials have also been used as stimuli responsive sensors for detecting the humidity, temperature, laser due to their unique localized plasmonic properties. However, traditional stimuli response plasmonic sensors are normally colloidal based, which make them hard to integrate with functional devices for real-world applications. This project can directly tackle this challenge by

designing and fabricating 2D soft responsive plasmonic sensors through self-assembly of plasmonic nanoparticles that functionalized by stimuli responsive polymers.

d) Flexible plasmonic electronics: This project aims to develop soft and flexible plasmonic electronic devices for electronic skin and bio energy devices. Traditional wearable electronics and biofuel cells are constructed with thick and rigid electrodes, which are not suitable for electronic skin and powering wearable electronics due to their poor mechanical compliance to curvilinear human body. This project can directly address this challenge by developing soft, thin yet stretchable conductor as gauge sensor or bioelectrodes via programming nanocrystal self-assembly.

e) Programmable binary plasmonic nanoassemblies (with Dr Robert Chapman): The collective properties of nanoassemblies can differ from individual building blocks or disordered assemblies due to the strong interactions between nanoparticles. While self-assembly of plasmonic nanocrystals into 2D nanoassemblies has shown semiconductor n/p-doping-like properties through controlled doping concentration,[2] the challenge lies in controlling the packing of the binary system with precise arrangement of different building blocks. In this project, we will integrate bottom-up self-assembly with stoichiometric reactions of complementary reactive polymers and/or DNA ligands to achieve programmable structural engineering of 2D binary plasmonic nanoassemblies. New polymers and DNA ligands will be synthesized in collaboration with Dr. Robert Chapman's group. We will synthesize plasmonic nanocrystals, functionalize them with the new polymers and DNA, and assemble them into highly ordered binary structures. Subsequently, we will characterize the plasmonic and structural morphology of these new assemblies using UV-VIS-NIR spectrophotometry, scanning electron microscopy, and transmission electron microscopy to investigate the relationship between their structure and properties.

Selected references:

1. D. Dong, R. Fu, Q. Shi, W. Cheng. Self-assembly and Characterization of 2D Plasmene Nanosheets. Nature Protocols, 2019. 14, 2691–2706.
2. Q. Shi†, D. Sikdar†, R. Fu, K. J. Si, D. Dong, Y. Liu, M. Premaratne, W. Cheng. Two-dimensional Binary Plasmonic Nanoassemblies with Semiconductor n/p-Doping-Like Properties. Adv. Mater., 2018, 30, 1801118.

Prof Erica Wanless

Polymers and Colloids at Interfaces

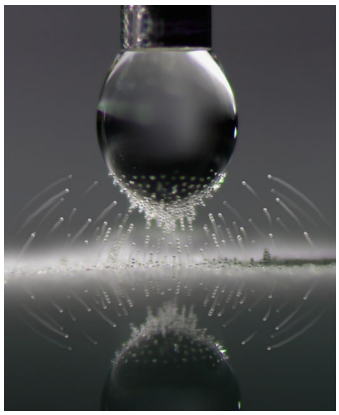
Website: https://www.newcastle.edu.au/profile/erica-wanless
Contact email: erica.wanless@newcastle.edu.au

Colloid chemistry is a form of materials science particularly concentrating on mixtures, where particles of one or more insoluble material are suspended within a dispersion medium. Surface chemistry is closely linked to colloid chemistry due to a focus on how the surfaces of these particles affect the physical and chemical interactions between the particles and the medium in which they are dispersed. The science of surfaces and particles is essential to food technology, the creation of personal care and cleaning products, as well as the enhancement of mineral separation, biomedical and other industrial technologies. Erica and her team are expert in designing and testing surface modifications to particles, as well as measuring the behaviours of particles at the phase boundary in new and existing colloidal dispersions.

a) Smart polymeric coatings: Polymer films can radically change the surface of a material while leaving the bulk properties of the material intact. The polymer surface coating controls the interaction with other objects through nanoscale forces. We will fabricate polymer films that contain an inbuilt molecular-scale switch from attractive to repulsive interactions, offering a means for dictating macroscopic character such as the wettability, adhesion or friction of a surface. Academic and industrial interest in these coatings is increasing rapidly, for potential application as low-friction coatings for confined parts or rheology modifiers. This project can have either a polymer synthesis, state-of-the-art physical chemistry characterisation (atomic force microscopy, ellipsometry etc), or materials engineering focus.

b) Unravelling specific ion effects: Specific-ion effects (those that depend on ion identity rather than simply salt concentration) are ubiquitous in industrial and natural processes, from next-generation lithium-polymer batteries to the chemical pathways that facilitate energy transfer in our cells and underpin life itself. Much can be gained by improving our fundamental knowledge of ion specificity and in particular, how surfaces and solvents interact with ions to impact the properties of soft matter and colloidal systems. The aim of this project is to conduct surface chemical investigations into how the properties of surfaces and solvents influence specific-ion effects and build our knowledge to ultimately predict and harness these curious effects. You will join the group experimental effort which is being complemented by Alister Page's simulations aimed at understanding the origins of these fascinating phenomena.

c) Electrostatic formation of liquid marbles: Liquid marbles are unique liquid-particle aggregates consisting of non-wetting particles coating and thus stabilising a liquid droplet core. These novel materials have inspired a variety of proposed applications, including pollution and gas sensors, actuators and microreactors. Until now, however, liquid marbles have been prepared one by one thus limiting their production and application. This project will study the formation of well-defined particle-stabilised liquid marbles using a novel electrostatic process. The expected outcome is a robust, repeatable process that can in future be scaled up to bulk production.



Three additional projects are available every year as part of the **ARC Centre of Excellence for Enabling Eco-Efficient Beneficiation of Minerals** led by the University of Newcastle. This Centre has a mission to reduce water usage and power consumption via smarter, more efficient mineral separation technologies including reprocessing of tailing stockpiles. Erica's role in this Centre lies in improving and optimising the adsorption of molecular and particulate components at the various interfaces that are the key to these technologies. You will join the greater team effort dedicated to more sustainable metal extraction for those 60+ metals in your smartphone!

d) Influence of hydrophobic particles on interfacial stability of emulsions and foams: Colloidal particles are alternative foam and emulsion stabilising agents to traditional surfactant molecules. In this project we will be investigating the interaction of foam bubbles or emulsion droplets using high speed video in order to understand the role that particles play in stabilising these interfaces. This is important to improving a range of technologies from collectors in mineral separation by flotation to emulsion binders in agglomeration processes. This project is a collaboration with Deakin University and the University of Adelaide.

e) Development of RAFT polymer collectors for selective flotation of specific minerals: This project seeks to design and develop novel RAFT-derived polymeric reagents as collectors for selective flotation of specific minerals. New polymers will be synthesised by collaborators at Monash University. At Newcastle we will characterise and quantify the adsorption of these new polymers at the phase boundary between various mineral surfaces with air and water in order to demonstrate selective and effective valuable minerals recovery.

f) Application of responsive synthetic and bio-polymers through reversible switching from hydrophilic to hydrophobic confirmations: In this project, which is being conducted with colleagues at Melbourne University, we will investigate the potential to improve the dewatering process in mineral tailings using conformational changes in added polymers adsorbed to particles to reversibly induce hydrophilicity or hydrophobicity as required. In this way we will facilitate the recovery of process water, which results in the reduction of the impact of mineral processing on the environment and significantly reduces the risks in tailings dam failures. At Newcastle, our experiments will focus on characterising polymer adsorption on gangue minerals and the contact angle that results.

g) Depolymerisation of plastic waste using polymer-coated enzymes *(with Dr Robert Chapman):* This project aims to design polymer coatings for enzymes that will enable them to be embedded into polyethylene, and later activated to in a compost heap to decompose the plastic to small molecules. See full description under Dr Chapman's profile.