CHEMISTRY

Academic Researcher:	Dr Lauren Macreadie
Project Title:	**Advanced materials for CO_2 reduction and water splitting catalysis**
Project Summary:	This project investigates advanced, framework materials as catalytic systems for water splitting and CO_2 reduction purposes. These materials are called metal organic frameworks (MOFs) and are the leading class of functional, porous material. This project will involve chemical synthesis and X-ray diffraction to understand the structure-property relationships for these systems.
Project Synopsis:	The rising global awareness in the devastating effects of high atmospheric levels of carbon dioxide (CO_2), coupled with a demand for transition from fuel-based transportation to a hydrogen based economy, has driven research toward decarbonization technologies. Decarbonization effects include transitions of processes reliant on fossil fuels to hydrogen fuel and the catalytic reduction of CO_2. Currently, fossil fuels are largely employed to create hydrogen gas, releasing atmospheric CO_2, which effectively negates the 'green benefits' of hydrogen fuel technology. Specialized catalysts can be used to meet these problems, however often catalysts used in industry lack recyclability. This project investigates metal organic frameworks (MOFs) as catalytic systems for two important purposes – water splitting and CO_2 reduction. The task of the PhD student is to investigate 2 separate systems, one system for water splitting to produce hydrogen in green methods, while the other system for CO_2 reduction to industrially important products. MOFs are ideal catalytic platforms as they offer a solid structural support for catalytic reactions and through judicious choice of organic ad metal components, their catalytic chemistry can be carefully tuned. To thoroughly investigate these systems, multiple techniques will be employed which will provide the successful candidate with an excellent suite of experimental knowledge. This includes organic synthesis, crystallography, neutron diffraction, synchrotron diffraction, and gas sorption
Additional Information:	This project is funded through an ARC DECRA at the University of Sydney, ranked 1st in Australia and 24th globally. It involves multiple collaborations with researchers in New Zealand, Germany (at the ARENA2036 institute) and the new VH2 hub at the CSIRO (Melbourne). The innovative nature of this work will allow the successful candidate to develop skills both in synthetic chemistry and in industrial collaborations, giving them an excellent platform for a future career post-PhD.

Academic Researcher:	Associate Professor Ivan Kassal
Project Title:	**Advanced organic electronics**
Project Summary:	This project aims to identify design rules for next-generation organic electronics, especially organic solar cells. It will use both computational simulations and experimental work to understand and improve organic electronic devices.

Project Synopsis:	How organic solar cells convert light into electricity is still not completely understood. The most perplexing aspect is why the positive and negative electric charges drift apart despite being strongly attracted to each other. This project will develop new simulation tools to better understand these fundamental processes, and then test them experimentally. The theory component will involve multiscale modelling to bridge the vastly different length scales that are important in organic electronics, all the way from atoms to full devices. Doing so will involve combining methods such as kinetic Monte Carlo with macroscopic drift diffusion models. The theoretical results will then be tested experimentally to confirm the predictions or provide data to refine them. The project can be tailored for the successful candidate to range from a focus on theoretical modelling of multi-scale processes to a mix of theory and experimental device study.
Additional Information:	Applicants should have a strong background in physical chemistry, chemical physics, or materials science, in either theory or experiment (or both).

Academic Researcher:	Dr Asaph Widmer-Cooper
Project Title:	**Using computer simulations to design better printable solar cells**
Project Summary:	The ability to print efficient, stable and cheap solar cells near ambient conditions would revolutionise our transition to renewable energy. Metal halide perovskites have emerged as a promising candidate for realising this dream, as a printable solar cell material with the fastest growing efficiency to date. The ARC Centre of Excellence in Exciton Science, in partnership with CSIRO, is working to make this a reality by combining a multidisciplinary research team with pilot-scale printing capabilities. In this project, you will use computer simulations to study how crystalline films of metal halide perovskites form from solution and how they are affected by moisture. The insights gained from this work will help our experimental partners to obtain better control of device nanostructure and performance. The Centre of Excellence in Exciton Science is funded by the Australian Research Council and links the University of Sydney, the University of Melbourne, Monash University, RMIT and UNSW, together with other national and international partners. As a PhD student in the Centre, you will be part of a network of over 100 students and scientists, with regular opportunities to take part in scientific meetings and training programs. For further information about the Centre. This project will include the opportunity to visit experimental collaborators in Melbourne.

Project Synopsis:	Metal halide perovskites are inorganic or organometallic materials that can be formed into thin crystalline films by depositing a solution of precursor ions onto a substrate and then removing the solvent. This process has been used to make very efficient perovskite solar cells (PSCs) at small scale, however there are barriers to converting this success into a mature technology. For example, PSCs are not as stable under humid environmental conditions as conventional siliconbased solar cells, and it is not currently possible to print efficient PSCs at scale. One of the central problems is that we lack a detailed understanding of how perovskite crystals form at the molecular level and of how to influence this process. To help solve this problem, you will use computational modelling to study the formation and dissolution of metal halide perovskites at the molecular level. This will involve the use of molecular dynamics simulations and statistical mechanics techniques to characterise the mechanism and thermodynamics of these processes, including the effect of changing experimental conditions. This will be done in close collaboration with experimental partners in Melbourne and with other members of our diverse research group at the University of Sydney. The expected outcome is a set of strategies (ink formulation and processing conditions) that can be used to print stable and efficient PSCs at scale.

Academic Researcher:	Dr Shelley Wickham
Project Title:	**A scalable, synthetic retina: signal processing in lipid droplet systems with DNA nanotechnology**
Project Summary:	This Australian Research Council funded project aims to develop externally-controlled DNA nanomachines for precision molecular communication across multi-compartment lipid droplet networks. The field of self-assembling DNA nanotechnology allows us to build programmable molecular nanomachines, which can be externally controlled by chemical, light, electrical and magnetic signals. The resulting DNA-lipid systems will have potential applications as 'organ-on-a-chip' models for high-throughput drug screening, synthetic tissue for medical implants and replacements, and neural and retinal prosthetics.

Project Synopsis:	Recent advances in machine learning mean that complex brain functions can be ‘read out’ and translated into external action, such as controlling robotic arms. However, we currently lack the necessary biotechnology to do the reverse, and ‘read in’ and translate complex external signals into biochemical functions. In this project we will take a synthetic biology approach, using engineering principles to repurpose or redesign biological components and systems to drive new applications. The student will repurpose DNA, proteins and lipids to design and build multi-compartment biomolecular systems and state-of-the-art nanotechnology to process external inputs (light patterns) and translate them into biochemical outputs (pH, membrane current, molecule transfer). The student will work with computational design tools to design new DNA nanostructures, then use experimental biochemistry techniques to assemble and purify them. Cutting-edge microscopy techniques such as cryo-TEM and super-resolution optical microscopy will be used to validate their functions. Electrophysiology experiments to show membrane signalling will then be done in collaboration with the Baker group at UNSW.
Additional Information:	This project is part of a collaborative ARC grant with Dr Matthew Baker (UNSW), Professor Hagan Bayley (Oxford, UK) and Dr Mike Booth (Oxford, UK), so may involve future travel opportunities to Oxford University in the UK. Excellent facilities are available to carry out all aspects of the work, including access to computing resources, electron microscopy and optical microscopy. The student should have a strong interest in synthetic biology or nanotechnology, and enjoy working as part of a vibrant interdisciplinary team. This project would suit a student with experience in experimental science (physics, chemistry, biochemistry, biology) or a quantitative background (physics, engineering, mathematics). Biochemistry experience is not essential. Top-up funding is available for the highest quality of applicants, with additional funding available to support travel to present research results at national and international conferences and to visit collaborators.

Academic Researcher:	Dr Girish Lakhwani
Project Title:	**PhD Position in organic semiconductor lasers**
Project Summary:	We are looking for a suitably qualified graduate student to work on a PhD project towards the advancement of a new kind of laser called polariton laser, which unlike conventional lasers can potentially operate at low input energy. The goal of this project is two-fold: firstly, to identify new materials that can demonstrate existence of half-light/half-matter quasiparticles called polaritons and secondly, demonstrate lasing action from these quasiparticles.

Project Synopsis:	Since the 1960s, lasers have transformed from an esoteric laboratory curiosity to a staple in everyday life, with presences in medical diagnostics, commerce, and material processing. As new applications emerge, each one brings new challenges, with specifications tailored to meet a specific objective. This has led to a large number of lasers with different properties, including wavelengths, linewidths, and output powers. However, for all applications, one specification is universal: the need for high efficiency. Increasing efficiency involves lowering the laser threshold, in other words, energy required to initiate laser emission. Traditionally, laser emission can only occur when more material is in the excited state than the ground state that unfortunately sets an effective upper limit on device efficiency. In this project, you will advance the development of a new kind of laser, known as polariton laser, which unlike conventional lasers can potentially operate at low input energy. Polaritons are half-light/half-matter quasiparticles that exist when a material placed in an optical cavity. The project will explore the fabrication and characterisation of polartion lasers using organic semiconductors such as fluorescent dyes. Device fabrication will include working in a cleanroom environment using glovebox with thermal evaporator and spincoater, while characterisation will include, not limited to angular reflection and fluorescence, time-resolved absorbance and imaging. The project will suit more to a student with a strong background in optical spectroscopy. The PhD student will join a multidisciplinary research team, with strong interactions with other research groups and institutions working under the ARC Centre of Excellence in Exciton Science (ACEx). The overall mission of the Centre is to examine and manipulate the way light energy is absorbed, transported and transformed in advanced molecular materials. Student will benefit from collaboration across Centre nodes, annual scientific seminars/meetings, and international partnerships.

Academic Researcher:	Dr Girish Lakhwani
Project Title:	**PhD Position in organic solar cells**
Project Summary:	We are looking for a suitably qualified graduate student to work on a PhD project towards the advancement of organic solar cells. The goal of the project is to understand the device function of organic solar cells and develop strategies to reduce current and voltage losses thereby providing design rules for highly efficient solar cells.

Project Synopsis:	Conjugated organic semiconductors have proven to be cheap, easily processable and flexible alternatives to silicon for sustainable energy applications like organic solar cells. Similar to photosynthesis, these materials funnel the absorbed sunlight to charge-transfer states where opposite free charges, electrons (-ve) and holes (+ve), are generated. These free charges must be transported to the respective electrodes and extracted to yield a flow of current. However, these opposite charges can sometimes find each other en route before reaching the electrodes and recombine due to Columbic attraction between them, resulting in a current loss. This tussle between charge transport and recombination influences the device efficiency drastically. This project aims at understanding device physics of organic solar cells and developing strategies to reduce charge recombination thereby providing design rules for highly efficient solar cells. Project will involve fabrication and characterisation of organic solar cells and performing transient spectroscopy to understand charge dynamics. Device fabrication will include working in a cleanroom environment using glovebox with thermal evaporator and spincoater. Characterisation of devices will involve recording and analysing current-voltage spectra, performing photocurrent decay measurements, using surface imaging tools such as AFM and TEM to image surface morphology and perform calculations to quantify the efficiency of electronic processes involved. This project is particularly of interest to students who are inclined towards physical chemistry and applied physics with focus on organic electronics. The PhD student will join a multidisciplinary research team, with strong interactions with other research groups and institutions working under the ARC Centre of Excellence in Exciton Science (ACEx). The overall mission of the Centre is to examine and manipulate the way light energy is absorbed, transported and transformed in advanced molecular materials. Student will benefit from collaboration across Centre nodes, annual scientific seminars/meetings, and international partnerships.