Project 1: Postgraduate Research Scholarship in Monolayer Two-Dimensional Materials

Keywords: two-dimensional nanomaterials; graphene; ionic liquids; neutron scattering

An opportunity is available for a PhD scholar to undertake research studies in the exfoliation and structure of monolayer two-dimensional materials. The aim of the research is to understand the mechanism of exfoliation and stability of dispersions of 2D materials in ionic liquid media.

In this project you will examine the nanoscale structure of 2D materials such as graphene and phosphorene as dispersions in ionic liquids, utilising advanced X-ray and neutron scattering techniques in our laboratory and at major international facilities. These techniques will be used to examine the molecular structure of the ionic liquids in bulk and at the surface of the dispersed 2D materials, revealing the factors that promote spontaneous exfoliation and stabilise the 2D structure. This new understanding will be used to improve the production rate and yield of exfoliated material, and thus to design conditions for their scalable and commercial production.

This project is part of a collaborative project with researchers at Monash University, the University of WA, and the Ecole Normale Supérieure de Lyon, and is funded by the Australian Research Council.

Supervisor: Professor Gregory Warr
School of Chemistry
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Project 2: Protein nanocompartments for advanced enzymatic catalysis

Keywords: chemistry, synthetic biology, protein engineering, synthesis, catalysis, enzymes

This project involves the chemical and biological modification of encapsulins, bacterial proteins that spontaneously assemble into hollow ~30 nm shells (see Nat. Commun. 2018, 9, 1311). A unique feature of encapsulins is their ability to house other molecules, in a targeted binding process that is mediated by a simple peptide tag. This project will involve creating nano-sized reaction vessels by functionalising the interior of these shells with synthetic molecules. These encapsulin compartments will then be probed in a range of functional assays to establish new applications in catalysis.

The project will involve expression and purification of engineered encapsulin nanocompartments. Different sequence variants from nature will be explored, and further designed mutations will be incorporated to tune the nature of the protein compartment. A range of enzymatic and non-native cargo will be explored. You will learn a broad range of techniques including protein production, HPLC/FPLC, peptide synthesis, and electron microscopy. There may also be the opportunity to conduct chemical synthesis, depending on how the direction of the project evolves over the course of the degree. In this project, we expect to gain a deep fundamental understanding of the encapsulin system, and translating this into catalytic applications demonstrating unprecedented selectivity, stability, and reactivity in engineered biological systems.

Applicants must have a background in chemistry, molecular biology, biochemistry, or synthetic biology. Applicants must also demonstrate a desire to build skills in organic chemistry, molecular biology, protein biochemistry and nanotechnology.

Supervisor: Dr Yu Heng Lau
School of Chemistry
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Project 3: Using computer simulations to design advanced nanoparticle inks

Keywords: nanoparticles, simulations, solar energy, ligands, self-assembly

Inorganic nanoparticles made of metals, semiconductors, and oxides are now used as functional components in sensing, photovoltaics, and light-emitting devices. The ARC Centre of Excellence in Exciton Science aims to use such nanoparticles to develop full spectrum solar energy conversion and more energy-efficient devices. In this project, you will use computer simulations to study nanoparticle inks, aiming to understand the molecular- and nano-scale origins of particle stability, shape and optoelectronic properties. This will help our experimental partners to obtain better control of device nanostructure and performance.

Nanoparticles are grown in solution and many applications require the particles to be dispersed in organic solvents or to pass through this stage during processing. Purely inorganic particles do not form stable dispersions in a polar solvents because van der Waals forces cause attraction and thus, agglomeration of the particles. Cores are therefore coated with organic molecules during synthesis or in later ligand-exchange procedures. The adsorbed ligands provide steric stabilisation, but can affect the particle stability, shape and optoelectronic properties in surprising and useful ways. For example, the ligands can undergo assembly into an ordered state that makes the particles attract one another, thus dramatically changing their colloidal stability. Ligands can also cause some types of nanocrystals to twist into chiral shapes, resulting in the formation of chiral assemblies with unusual optoelectronic properties. In addition, dye molecules can be attached to the nanocrystal surface, which can be used to change the absorption and emission properties of the particle. You will use detailed molecular dynamics simulations and statistical mechanics techniques to investigate the microscopic forces responsible for this diverse range of behaviour, as part of a lively research group at the University of Sydney. This will be done in close collaboration with experimental partners in Melbourne and Europe.

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 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, see https://excitonscience.com. This project will include the opportunity to visit collaborators in Melbourne and in Europe. Applicants must have a strong background in physical chemistry, chemical physics or a related field. Strong mathematics skills and programming experience would be an advantage. Previous experience with computer simulations is desirable.

Supervisor: Dr Asaph Widmer-Cooper
School of Chemistry
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Postgraduate Research Excellence Award
in the Faculty of Science

Project 4: Quantum Error Correction and Tensor Networks

Keywords: quantum error correction; quantum computation; tensor networks

This project will seek to understand quantum error correction, which concerns itself with the reliable storage and processing of quantum information on a quantum computer, using tensor networks, which are a tool for studying quantum many-body systems. Without quantum error correction, quantum computers will never be able to unlock their full potential. Reducing resource overheads for error-correction schemes will be of increasing importance over the next coming years as the first small-scale quantum devices are entering the market.

The project will proceed as follows. We will investigate quantum error correction and tensor networks via the following steps:

0. Study background on a special type of tensor network known as MERA.
1. Define a new modification of MERA that will make the tensor network simulation amenable to a near-term quantum device.
2. Analyze the noise resilience for the tensor network.
3. Investigate whether the contraction algorithms appearing in the prior literature naturally carry forward to the new tensor networks defined in the project.
4. Compare this near-term quantum algorithm with the best known classical algorithms and via benchmarking through numerical simulations.

The expected outcome is a new class of tensor networks that may be useful for decoding quantum error correcting codes with lower resource overheads.

Supervisor: Professor Steven Flammia
School of Physics
View this project on Research Supervisor Connect

Additional Supervisor: Professor Stephen Bartlett
Project 5: Ground-state cooling and high-fidelity detection of large ion crystals in a Penning trap for quantum simulations

Keywords: quantum simulation, ion trapping, atomic physics, laser systems

The understanding of the dynamics of many-body quantum systems is one of the most challenging problems in physics today. Advancing our knowledge of these systems can lead to significant benefits in the understanding of condensed matter phenomena such as high-temperature superconductivity and spin liquids but also enable insights into dense astrophysical matter as found e.g. in neutron stars. To gain controlled access to these systems and engineer their interaction, we are using some of the most precise tools in atomic physics, the Penning ion trap and laser systems, to build and investigate multi-particle systems ion by ion.

The controlled simulation of dynamics in quantum-many body systems is of central interest in the pursuit to further our understanding of condensed matter phenomena. Specially designed Penning ion traps enable experimental investigations into these topics using hundreds of ions trapped simultaneously. We have recently brought online the first and only such system in Australia at the Sydney Nanoscience Hub and now routinely trap large crystals of beryllium ions. The focus of the work is on finalizing the setup of the laser-based beryllium qubit manipulation and implementing software-based state analysis. Lasers near 313nm are used to address electric dipole transitions in beryllium ions. These transitions can be used to effectively Doppler laser cool an ensemble of ions to ~1mK temperature, such that it forms an ion crystal - a regular and stable lattice of charged particles, formed due to the equilibrium of Coulomb repulsion and electromagnetic confinement. However, for many envisaged experiments, the residual motional temperature has to be decreased even further, close to the ground state of motion. This can be achieved by implementing so-called ground state cooling techniques using lasers with different beam geometry and characteristics. The development and setup of this system, followed by the before mentioned state-of-the-art quantum simulation and metrology experiments is a possible project. To investigate correlations between individual ions, or qubits, in a quantum simulation, the spin state of the ion has to be read out. This is accomplished by detecting the ion’s fluorescence photons. Ion crystals in a Penning trap rotate in the strong external magnetic field of a superconducting magnet due the Lorentz force. Therefore, a precise correlation between photon time an position is required. The setup of such detection systems and its integration into the existing experimental control software in combination with the development of algorithms employing machine learning is a possible project. These projects are expected to generate new knowledge in the area of quantum science and have a multitude of possible future applications in quantum technology, such as quantum scale materials, quantum sensing and quantum computation. In particular, understanding quantum magnetism is on the forefront of modern physics.

Supervisor: Dr Robert Wolf
School of Physics
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Additional Supervisor: Professor Michael Biercuk