



Australian Centre for Neutron Scattering ECR Clip Day 2021

Abstract Booklet | 25 - 26 February

Hosts: Oliver Paull, Sam Yick & Kathleen Wood

Comparing inelastic neutron scattering with theory to understand the complex magnetic interactions in a low-dimensional frustrated magnet

Frustrated magnetic systems have gained a lot of recent interest as they can exhibit exotic magnetic quantum states such as spin-liquid and spin-nematic states [1,2]. The natural mineral atacamite, $\text{Cu}_2\text{Cl}(\text{OH})_3$, is one such material, showing behaviour characteristic of a frustrated magnet [3].

This work studies this lesser understood polymorph of orthorhombic atacamite, where Cu^{2+} ions form a pyrochlore lattice. The novel magnetic interactions and quantum states in materials like atacamite lends itself to spintronic applications where understanding spin interactions can unveil opportunities for intentionally manipulating these spins.

Time-of-flight inelastic neutron scattering measurements on single crystalline atacamite have been performed at Pelican. Excitations were observed at 1.5K, and weakened as temperature was increased beyond the antiferromagnetic transition temperature of $T_N=9.0\text{K}$ [4] to 20K. The strongest dispersion was found along the H00 direction with relatively weak dispersion along 00L, and a flat mode was observed in out-of-plane scattering covering a narrow section in 0K0.

Ab initio band structure calculations have indicated a 1D sawtooth chain model for the dominant magnetic exchange paths in atacamite [5].

However, the relative magnitudes of the predicted exchange couplings appear counterintuitive with respect to the strongest dispersion measured experimentally in the H00 direction. Is the theoretical model flawed, or is there another explanation for the discrepancy of exchange couplings? Finally, to better understand the interactions in atacamite, in-field time-of-flight measurements have also been conducted in magnetic fields up to 6.5T. Data were collected using Pelican and the new open geometry, fully compensated, 7T vertical magnet.

References:

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- [3] X.G. Zheng et al. Phys. Rev. B 71, 174404, (2005)
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- [5] L. Heinze et al., arXiv:1904.07820 (2019)

Bio of presenting author

I come from Ulladulla, a small town on the South Coast. I came up to Wollongong in 2016 to start studying physics at University. In 2019 I began my honours year of my physics degree, looking at terahertz spectroscopy of amino acids. Now, I'm starting my second year of my PhD at both the University of Wollongong and ANSTO, with Roger Lewis and Kirrily Rule as supervisors, respectively. My main project aims to look at the magnetic structure of a frustrated quantum magnet, atacamite.



Jackson Allen

University of Wollongong

Academic Level
PhD (2nd year)

ACNS Co-supervisor
Kirrily Rule

Neutron scattering for the study of real-time devolution of casein gel microstructure during in situ enzymatic digestion and enzyme diffusion

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The structure of food largely determines the kinetics and extent of food digestion and thus nutrient absorption. As disruption of the food matrix upon digestion will strongly regulate bioaccessibility of nutrients, understanding the role of structural modification of food on digestibility will provide a strategy towards modifying the food matrix with particular nutrition and health benefits for the delivery of personalized nutrition.

In our previous ultra-small and small-angle neutron scattering study, casein gels with identical composition but differing by the coagulation mode, were submitted to simulated in vitro gastric digestion and digesta products were collected after 15 and 120 min exposure to the simulated gastric digestion. However, it is well known that microstructural changes in food during digestion is highly time-dependent. Therefore, in situ monitoring of structural changes during digestion is a major topic of interest that offers many advantages to understand the behaviour of complex food systems. Using an in situ digestion setup, where the digestion chamber was connected to a pump at the bottom of the vessel to pump the gel particles through the cell, the kinetic effects of mechanical deformation during a 2-hour digestion was monitored at as short as 5 min intervals for multiple time points using the Bilby beamline in time-of-flight mode and Kookaburra beamline.

Furthermore, it is well known that protein digestion is mostly influenced by pepsin activity which has a limited penetration depth within samples. To understand the diffusion of digestive enzymes within food microstructures in more detail, we studied diffusive motions of water within the initial and digested gel as the structure changes using Quasi-elastic neutron scattering (QENS).

Our findings will provide a fundamental understanding of the factors causing resistance or susceptibility to the disintegration of casein matrices under simulated gastric digestion.

Bio of presenting author

I am a second year PhD student at CSIRO Agriculture and Food Centre and RMIT University. My research investigates the evolution of food structures within food matrices upon digestion. I hold an MSc in Food Science from the University of Melbourne and a BSc in Molecular Biology and Bioengineering from Sabanci University (Istanbul, Turkey). I was recently selected for Homeward Bound, a global leadership program for women in STEMM.



Meltem
Bayrak

RMIT

Academic Level
PhD (2nd year)

ACNS Co-supervisor
Jitendra Mata

Design and synthesis of an azobenzene-betaine surfactant for photo-rheological fluids

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Photo-rheological fluids (PRFs) are materials that modulate their flow properties, such as viscosity and elasticity, when exposed to light of a specific wavelength. The unique stimulus-responsive properties of PRFs, driven by control of nanoscale surfactant aggregates, gives them potential for application in microfluidics, mineral extraction, bioseparations, drag reduction and templated synthesis. Most PRFs comprise a mixture of surfactants, additives and salts, in order to elicit the desired stimulus-responsive rheological properties, however, development of more simple, robust and effective systems is a necessity for their broad uptake and integration of such chemistry.

Our work has centered around the development of a novel azobenzene containing surfactant, capable of forming a PRF without the need for any additives, salts or co-surfactants. Irradiation of the aqueous solution state molecule results in switching of the surfactant aggregates from entangled wormlike micelles to discrete ellipsoidal aggregates, accompanied by concomitant changes in zero-shear viscosity up to 16,000 \times (Fig. 1).

These experiments reveal fundamental and previously unexplored structure-function relationships of azo-surfactants and demonstrate the power of molecular design in realising novel colloidal materials with stimulus-responsive, switchable properties.

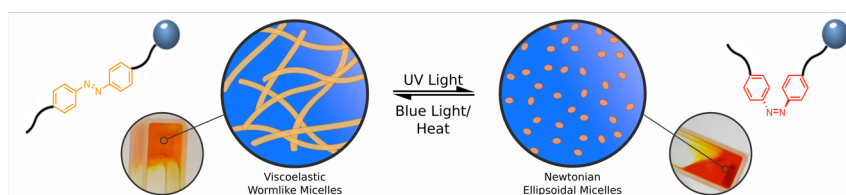


Figure 1. Schematic showing transition from viscoelastic wormlike micelles to inviscid ellipsoids upon isomerization of an azobenzene containing surfactant

Bio of presenting author

I completed my honors in synthetic chemistry before moving into interfacial and colloidal science for my PhD at Monash University. My research focuses on establishment of structure function relationships and synthesis of novel surfactants. In my spare time I like to play guitar and ride my bike.



Calum
Butler

Monash University

Academic Level
PhD (3rd year)

ACNS Co-supervisor
Anna Sokolova

Elucidation of the wave function of the ground doublet in a Tb complex using INS in a magnetic field

Lanthanoid Single Molecule Magnets (SMMs) are molecular materials that exhibit slow relaxation of the magnetisation of molecular origin, thus showing promise for a wide range of technological applications which include spintronic devices and molecular memories. The interaction between the atomic lowest-lying spin-orbit multiplet of the LnIII ion and the electron density of the ligands weakly splits the former into a set of crystal field states. Since this splitting is significantly weaker than other energy contributions in lanthanoid complexes, the details of the interaction between the electron densities of the LnIII ion and of the ligands are crucial for the development of SMMs which can operate at high enough temperatures to warrant widespread practical applications.

It is crucial, therefore, to understand in detail how the crystal field interaction influences the relaxation of LnIII SMMs, and to this end joint experimental and computational and theoretical methods effort has proven to be very useful, in that (i) theoretical results provide a rationalization of experimental results, thus being routinely employed in the molecular magnetism literature, and (ii) comparison of theoretical simulations with different experimental measurements can showcase the shortcomings of the specific theoretical or computational approach utilised, providing a rationale on the improvements to introduce in order to improve their ability to successfully describe the properties of the system.

Previously, we have performed Inelastic Neutron Scattering (INS) measurements on the complex $[\text{Tb}(\text{bpy})_2(\text{Cl}_4\text{Cat})(\text{Cl}_4\text{CatH})(\text{MeOH})]$ using the PELICAN instrument, where we observed a shoulder to the elastic line which, after fitting, was established to arise from a single transition. While theoretical calculations of the low-lying energy spectrum of the complex were able to rationalize the observed transition as arising from quantum tunnelling within the ground Ising doublet, the tunnelling gap predicted by such calculations is significantly smaller than the one which has been experimentally determined, thus highlighting the inability of such calculations to correctly predict the electronic properties of the ground state of the molecule.

In this study, therefore, we have measured the INS spectra for the aforementioned complex, under the same experimental conditions of the previous experiment, employing the newly commissioned 7 T magnet on PELICAN, where we predicted that the evolution of the observed transition in an increasing magnetic field would allow us to obtain relevant information on (i) the electronic properties of the ground state and (ii) the nature of the magnetic transition observed in the zero-field spectrum. The measurements show that, with increasing magnetic field, the INS transition (i) becomes less intense, thus confirming that the observed peak arises from the quantum tunnelling of the ground state, and (ii) splits into multiple peaks, both as a result of the usage of a powder sample and the complex spin-orbit composition of the wave function of the ground Ising doublet.

Bio of presenting author

Dr. Simone Calvello has graduated cum laude at the University of Modena and Reggio Emilia. Afterwards, he moved to Australia to undertake a PhD under A./Prof. Alessandro Soncini at the University of Melbourne, where he contributed to the development of a novel methodology for the calculation of the electronic structure of lanthanoid complexes and to its implementation in a new software. Simone has just completed a Postdoctoral Fellowship under the supervision of A./Prof. Alessandro Soncini and Richard Mole at ANSTO, in which he studied the electronic and magnetic properties of promising lanthanoid complexes



Simone Calvello

University of Melbourne

Academic Level ECR

ACNS Co-supervisor Richard Mole

Heavy Starch: Biosynthesis and characterization of fully deuterated glucans

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For the first time, starch biosynthesis in genetically modified yeast has been used to produce deuterated starch by growing the yeast in deuterated media. The structure of starch granules consists of lamellar repeats of semicrystalline amylose helices which alternate with non-crystalline amylopectin layers. Current methods only deuterate the outer starch granule structure or destroy the layered granular structure entirely. Our methods of deuteration targeted the entire structure of the granule, keeping the layers in-tact. Due to the reduced scattering length density of deuterium as opposed to hydrogen, deuteration of the whole starch granule allows for an entire suite of new starch SANS experiments to take place, as well as new NMR and digestion kinetics experiments which could further elucidate the complex structure of starch and its role in biochemical systems.

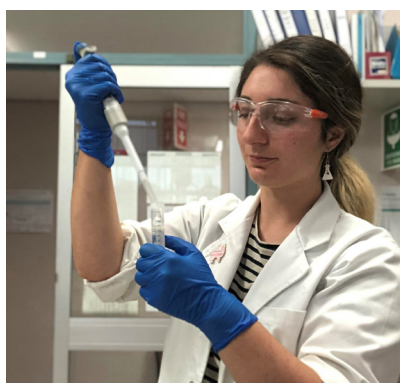
The genetically modified yeast strain used in this experiment (supplied by Barbara Pfister, ETH, Zürich) was grown from agar plates into large volumes of growth media, which usually consist of simple sugars, yeast extract, and proteins in water, to provide the yeast with everything it needs to grow. Our yeast cultures were grown in either 100% D₂O instead of H₂O, or in H₂O with deuterated raffinose as opposed to the regular protonated galactose sugar. Once grown, the yeast cells were lysed and the starch was collected, purified, and analyzed.

FTIR and SEM were used to confirm the starch product, with the “fingerprint region” of the collected FTIR spectrum matching those of commercial starches, and the SEM images matching those reported by Pfister et al. It was noted that the FTIR spectrum could not be used to detect any deuteration, as the expected C-D peak was not observed, likely due to the complex nature of the granules. Mass spectroscopy results on amyloglucosidase-digested samples showed that both D₂O methods and deuterated raffinose methods yielded deuteration to some degree at non-exchangeable positions, which is surprising considering the biochemical pathway for the production of starch is not currently thought to involve the incorporation of water. This could mean that the currently accepted model for starch biosynthesis will need to be reevaluated.

Upcoming work on this project will involve the use of deuterated starch samples in SANS and NMR experiments at ANSTO and UNSW for further characterization.

Bio of presenting author

After taking a term off from my lab-heavy research due to COVID restrictions, I’m wrapping up my final term of my Honours thesis at UNSW/ANSTO. I love working in the lab, and I hope to focus on a hands-on career path. I have a side interest in geology, and I can’t go anywhere without talking about the rocks! I’ve recently moved to Canberra with my fiancé, where I will soon be looking for my first full-time role.



**Lillian
Caruana**

University of
New South Wales

Academic Level
Honours student

ACNS Co-supervisor
Elliot Gilbert

New insights into colloidal phase transitions using neutron scattering techniques

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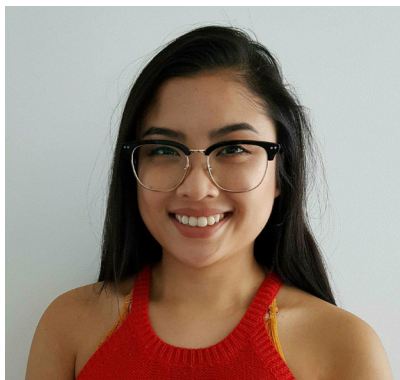
2 Malmö University, Malmö, Sweden

The fundamentals of crystallisation and glass formation in atomic systems are not yet fully understood. Colloidal nanoparticles have been shown to be promising model systems for understanding crystallisation and glass formation in atomic systems: As colloidal motion is Brownian, rather than ballistic, kinetics and dynamics are orders of magnitude slower than in atomic systems and can be studied in real-time. However, despite previous work, key elements are still missing from our understanding of phase transition in colloidal suspensions especially regarding metastability, supercooling and the glass transition. In particular, there is still no clear understanding of the effects of polydispersity: although studies of both polydisperse and binary mixtures of hard sphere colloids have been performed, a systematic study of the effects of polydispersity on structure, crystallisation kinetics and particle dynamics is still lacking.

One of the reasons for this is the relatively limited types of suspensions which have been studied - most particles used for such studies need to be suspended in mixed solvents for refractive index matching for light scattering studies, which introduces potential problems such as selective solvation and evaporation. In this work we explore the possibility of using ionic liquids (ILs) and deep eutectic solvents (DESs) as the suspending solvent, as these can be tuned to match the refractive index of the particles, and don't suffer from evaporation. We will then develop suitable binary colloidal suspensions consisting of deuterated & non-deuterated nanoparticles suspended in the solvent. With a combination of lab techniques and beam time allocations at the Australian Synchrotron, ANSTO and overseas neutron facilities, we will expansively investigate the nature of metastability, crystallisation and the glass transition, and provide a significant advance on our current understanding of these processes.

Bio of presenting author

I did my Honours at RMIT University and will be continuing onto my PhD. I have experience in using neutron scattering techniques to probe condensed matter materials, and for my PhD I intend to use neutrons to probe soft matter systems. I play badminton and sing in my spare time.



**Katherine
Chea**

RMIT University

Academic Level
PhD (1st year)

ACNS Co-supervisor
Jitendra Mata

Characterization of insect odorant receptor nanodiscs for detection of odorant compounds

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Insect odorant receptors (iORs) are membrane proteins in olfactory neurons of insect antennae enabling highly sensitive detection of odorant molecules. This makes iORs ideal candidates as bio recognition elements for developing biosensors with potential applications in food industry, biosecurity and pest control. Or22a from the fruit fly *Drosophila melanogaster* was used as a model receptor for the study.

iOR nanodiscs covalently immobilized on a gold substrate were characterized by atomic force microscopy (AFM), quartz crystal microbalance with dissipation monitoring (QCM-D) and neutron reflectometry in order to study surface modification and understand the underlying mechanisms associated with ligand binding. The EIS sensor exhibited high sensitivity and specificity towards ethyl hexanoate with a detection limit of 5.5 fM. Neutron reflectometry studies provided evidence to support conformational changes in the receptor upon ligand binding.

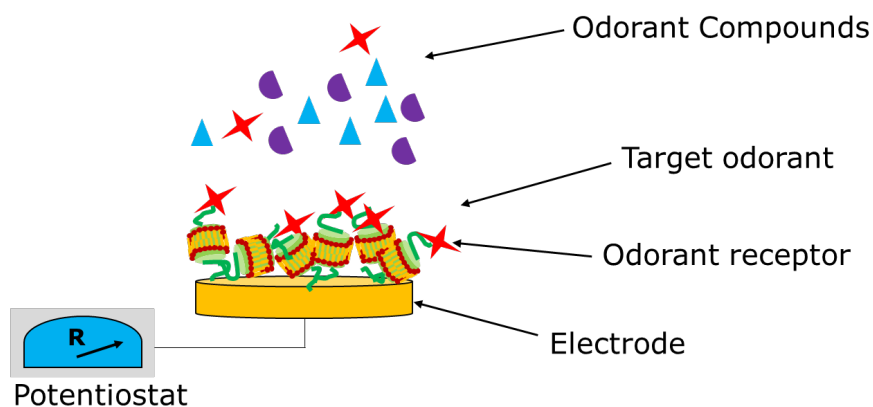


Figure 1: Schematic of the proposed electrochemical biosensor

Bio of presenting author

I did my MSc research at the Nanyang Technological University and currently pursuing my PhD at the University of Auckland. The PhD research involves developing insect odorant receptor based biosensing strategy.



**Jamal
Cheema**

University of Auckland

Academic Level
PhD (3rd year)

ACNS Co-supervisor
Andrew Nelson

Investigating anaerobic granules for enhanced self-healing concrete in wastewater infrastructure

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The phenomenon of self-healing in terms of microbial induced calcite precipitation (MICP) has been disclosed largely in the past few decades in response to the increasing awareness for the safety and sustainability of concrete structures. The efficient bonding capacity and compatibility with the concrete compositions attracted the interest of researchers. Recent studies investigated the application of various axenic microbial cultures coupled with protective carriers for developing self-healing bioconcrete. Despite the remarkable progress achieved to date, the high costs involved in the cultivation and encapsulation of the axenic cultures have led to a shift of research focus on the use of non-axenic microbial cultures. They have superior benefits as self-healing agents in terms of easy cultivation and low cost. Considering the high need for concrete-based wastewater infrastructure, novel, self-protected granules of sulfate-reducing bacteria (SRB) and nitrate-reducing bacteria (NRB) are being cultivated in an upflow anaerobic sludge blanket reactor by growing SRB and NRB on organic substrates from wastewater which further reduces the need for the addition of other nutrients. The bioconcrete is proposed to be achieved by mixing these granules into the general-purpose concrete. If concrete damage occurs, the bacteria will be activated to carry out the MICP by using the organic substrates from wastewater to autogenously heal the cracks. It is being anticipated that the proposed project will enhance the self-healing efficiency of bioconcrete by sealing the cracks of width $\sim 500\mu\text{m}$. To visualize the results of the project, the neutron imaging facility DINGO at ANSTO will be the most important equipment as it helps in observing the deeper layers of the specimens without destroying them. In addition to their strong penetration power, neutrons are sensitive to any hydrogen containing material like organic water or bacteria. First measurements have been analyzed by TomoPy for 3D-reconstruction and VGStudio for 3D-rendering and segmentation.

Keywords: Self-healing, Bioconcrete, Axenic cultures, Non-axenic cultures.

Bio of presenting author

I did my Master of Technology in Biotechnology at the Jawaharlal Nehru Technological University, Hyderabad, India. Currently, I am a PhD student at the University of Wollongong, working on developing a self-healing concrete. I am a trained Indian classical dancer and love travelling.



**Kirthi
Chetty**

University of
Wollongong

Academic Level
PhD (1st year)

ACNS Co-supervisor
Ulf Garbe

Diffusion in modified solid-state ionic conductors for energy applications: towards a complete picture from structure and dynamics

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The poor ionic conductivity of solid-state electrolytes compared to their liquid counterparts has prevented the widespread implementation of all solid-state batteries. A strategy that has been widely used to address this issue is the modification of solid-state ionic conductors via chemical doping. However, the complex resultant structures and the presence of secondary phases have meant that understanding how the improved ionic conductivity is achieved remains a challenge.

This work presents a strategy for characterizing solid-state ionic conductors using combination of neutron powder diffraction (NPD) and quasi-elastic neutron scattering (QENS) through a case study of Mg-doped NASICON and its secondary phase $\gamma\text{-Na}_3\text{PO}_4$. These materials are each representative of vastly different structure types, with NASICON featuring a rigid 3D skeleton framework that facilitates the passage of sodium cations through wide interstitial channels whilst, $\gamma\text{-Na}_3\text{PO}_4$ is a rotor phase material with a densely packed lattice. The differences in structure are reflected in their respective sodium diffusion processes.

In this presentation, the relationship between these two phases in the Mg-doped NASICON system will be discussed. A model of the Na^+ self-diffusion mechanism in $\gamma\text{-Na}_3\text{PO}_4$ which highlights the influence on the dynamics of the framework structure on ionic diffusion will also be shown. The strategies employed demonstrate a holistic approach to characterizing complex structures which can also be applied in a broader context.

Bio of presenting author

I did my Honours research investigating quantum electronic transport in semiconductor devices. For my PhD, I jumped fields to investigating the structure and diffusion processes in energy materials. By the time of the ACNS Clip day, I should have just submitted my thesis!



Emily
Cheung

University of
New South Wales

Academic Level
Other

ACNS Co-supervisor
Nicolas de Souza

Membrane thinning effect on bacterial membrane by linear lipopeptide battacin

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Linear form of antimicrobial peptide battacin had been discovered to be more active on bacterial membrane compared to its cyclic form but information about the mechanism of action of the peptides is still scarce.¹ Deformation of the membrane through membrane thickness is a common intermediate action for antimicrobial peptide.² We have been tried to probe this effect as an initial point to understand the interaction between the peptide and the membrane using Electrical Impedance Spectroscopy (EIS), molecular dynamic (MD), and Small angle neutron scattering (SANS).

Our results indicate that the peptide with longer alkyl chain (myristyl) can induce membrane thinning on the bacterial membrane. However, we face several difficulties to obtain quantitative data from our SANS measurement. Thickness value from kratky porod plot is thinner than MD measurement and what had been reported in the literature. Fitting process become more challenging with the presence of an additional broad peak in the lower q region of the scattering plot. Challenges to measure the thickness of the membrane using liposomes model system through SANS will be discussed during the presentation.

References:

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2.Grage, S. L.; Afonin, S.; Kara, S.; Buth, G.; Ulrich, A. S., Membrane thinning and thickening induced by membrane-active amphipathic peptides. *Frontiers in cell and developmental biology* 2016, 4, 65.

Bio of presenting author

I have completed my undergraduate study and Honours at University of Auckland supported by MARA, Malaysia. Currently, I am in my third year of my PhD studies at the same university. My research project is revolving around mechanism of action of antimicrobial peptide and funded by MacDiarmid and AINSE.



**NUR MAIZURA
DARBI**

The University of
Auckland

Academic Level
PhD (3rd year)

ACNS Co-supervisor
Anna Sokolova

Quatros Amigos- the four stromatolites in a row. The first 3D image of the oldest evidence of life in the geologic record

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*lead presenter

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The 3.48 Dresser Formation, Pilbara Craton, Western Australia provides the Earth's most convincing evidence of early life through a diverse array of biosignatures; including: domical, wrinkly, and coniform stromatolites, fractionated carbon, sulphur isotopes, biological organic-matter remnants, trace element distribution patterns, and hot spring deposits with microbial textures. However, identifying biosignatures in Archean rocks is difficult due to billions of years of erosion, deformation, and metamorphic alteration. Characterisation of community-accepted biosignatures also remains challenging, particularly the robustness of textural biosignatures as indicators of early life in Archean rocks. The textural biosignatures identified in the Dresser Formation are identified in surface outcrops that are weathered to 10's of metres depth. Therefore, in May 2019, fresh Dresser deposits were drilled to aid in a better understanding of these ancient biosignatures and to provide validity to a biogenic origin.

3 unweathered cores of 5-30 m thickness and 8 cm in diameter were extracted from ~70 m beneath the land surface. The cores provide excellent preservation of biosignatures, including the preservation of fossilized, pyritized, stromatolites. One stromatolite horizon within the core exhibits extraordinary morphological structures. Here we present preliminary results of the 3D geometry of these fossil stromatolites. 3D structures were obtained using the neutron imaging station DINGO at ANSTO. A full tomography of a first sample has been scanned with 1896 projection with an angular step of 0.19° and an exposure time of 60 seconds per projection. The data was reconstructed using filtered backprojection technique with tompy (a free python toolbox). 3D-rendering and segmentation was done with VG-Studio. This horizon aids in better defining the biogenicity of these textural biosignatures.

Bio of presenting author

I am a PhD student at the University of Auckland in New Zealand. My research looks at the earliest evidence of terrestrial life on Earth in 3.5-billion-year-old and possible life on other planets, such as Mars. I love the outdoors and travel, and often go for hikes or scuba diving in my free time.



**Michaela
Dobson**

The University of
Auckland

Academic Level
PhD (2nd year)

ACNS Co-supervisor
Ulf Garbe

From plastic crystals to orientational glasses- the role of disorder in hybrid perovskites + image

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*lead presenter

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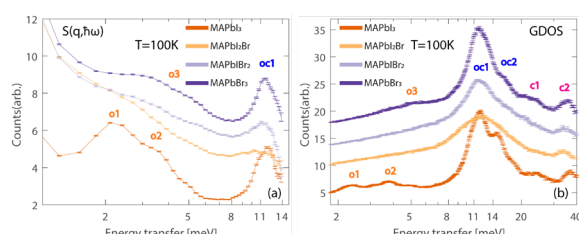
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Lead halide hybrid perovskites are known as solution processable, cheap photovoltaic materials that achieve high power conversion efficiencies. While the low-cost manufacturing being the driving mechanism for their research boom in the last decade, they still face a challenge of commercial application due to their instability under the light and atmospheric conditions. The best perovskite solar cells today are made by alloying, i.e. either mixing multiple cation components or including multiple halide atoms in the perovskite framework. However, the physics behind the success is still not well understood which limits further advancement. We choose both mixed and pure halide systems and pursue a detailed investigation of both phononic and molecular dynamics properties at ANSTO.

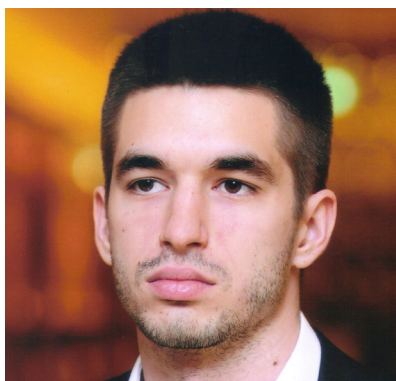
By using PELICAN we show that apart from the structural phase transitions that exhibit different behavior between mixed (MAPbI₂Br, MAPbBr₂) and pure halide perovskites (MAPbBr₃, MAPbI₃) there is also a disorder transition present in the lattice, i.e. from the high temperature plastic crystal phase to the low temperature orientational glass phase. This is observed in measured phonon density of states (pDOS) as a phonon melting phenomena. In the figure bellow, we emphasize the differences in the disorder transition behavior between inorganic octahedra (o1, o2, o3), inorganic-organic (oc1, oc2) and purely organic (cation) phonon modes (c1, c2) for both mixed and pure crystals.



We further carry out time resolved photoluminescence measurements and ultrafast transient absorption spectroscopy to determine the correlation between dynamic disorder and optoelectronic properties, with the aim to shed light on the origin of the improved photovoltaic performance of mixed halide perovskites.

Bio of presenting author

I did my undergraduate and master studies at the University of Belgrade, Serbia and I am currently doing PhD at UNSW, with my research topic being spectroscopic methods for investigating dynamic processes in hybrid perovskites.



**Milos
Dubajic**

University of
New South Wales

Academic Level
PhD (3rd year)

ACNS Co-supervisor
Kirrily Rule

Inelastic neutron scattering of lanthanoid-radical complexes

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Single-molecule magnets (SMMs) are materials which exhibit slow relaxation of magnetization and quantum tunneling of molecular origin, properties which make them promising for applications in high-density data storage, or as qubits in quantum computing.¹ The best performing SMMs are complexes of the late trivalent lanthanoid (Ln(III)) ions, where the energy barrier to reversal of magnetization stems from the crystal field (CF) splitting of the spin-orbit coupled ground state. Additional incorporation of organic radicals can be used to modulate SMM behaviour. Crystal field splitting and magnetic exchange coupling in these systems can be hard to determine using traditional magnetometric techniques; however, inelastic neutron scattering (INS) is a powerful experimental technique for directly measuring this splitting in Ln(III) compounds.²

Our group has been studying a family of compounds with formula [Ln(dbsq)Tp2] (Figure 1) which show exchange coupling between the Ln(III) ion and the dbsq organic radical.³ We have studied the INS spectra the Ln = Tb, Ho, Er and Yb analogues on the cold neutron time-of-flight spectrometer PELICAN, as well as their magnetic properties. We observe temperature dependent CF transitions, which are compared to the energy level splitting obtained from electronic structure calculations. Exchange transitions are also observed in some analogues, giving the first systematic study of Ln-radical exchange coupling in a molecular system.

Figure 1: [Ln(dbsq)Tp2] (left) and CF transitions of the Ho(III) analogue (right).

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Bio of presenting author

I did my Masters research at the University of Melbourne under the supervision of Colette Boskovic in the field of Ln(III) single molecule magnets. I am currently undertaking a PhD in the same group, studying exchange-coupled Ln(III) molecular compounds in collaboration with Richard Mole at ANSTO and with the support of AINSE.



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Cooperative Enhancement of Catalytic Activities in Ternary Compounds for Solar Thermochemical Ammonia Synthesis

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Ammonia is an indispensable industrial material that acts as a precursor for large-scale manufacturing of many essential products including agricultural fertilizers, pharmaceutical drugs, and explosives. Recently, it has also been proposed as a viable solution as hydrogen carrier due to its easily liquefiable nature and the existing global distribution network. The most mature method for producing ammonia in industrial scale is the Haber-Bosch (HB) process, which catalytically converts nitrogen and hydrogen into ammonia at elevated pressure and temperature. However, this century-old process is heavy in both energy consumption and greenhouse gas emissions, particularly when energies are sourced from the combustion of fossil fuels. Tremendous effort has been made to either ameliorate the traditional HB process or explore new methods. Among all the newly proposed synthetic routes, solar thermochemical ammonia synthesis (STAS) based on cyclic reactions between metal oxide and metal nitride holds tremendous promises for the future of ammonia industry, which sustainably produces ammonia from naturally abundant resources, such as sunlight, water, and nitrogen. Herein, to discover new, effective, and cheap solid-state catalysts for STAS, we applied a machine-learned temperature-dependent Gibbs free energy descriptor to screen 1439 ternary oxide/nitride pairs with their complementary binaries. More specifically, inspired by the concept of 'cooperativity', which was traditionally used in judging the stabilisation/destabilisation effects from noncovalent interactions in molecular systems, we applied it to examine whether the ubiquitous metal-metal interactions in ternary metal oxide catalysts can indeed enhance the reactivity compared to their complementary binaries. The results have shown that the cooperative enhancement effect is observable but rare. We envisage that the work presented in this study will open new pathway to understand the operating principles behind solid-state catalysts in the future.

Bio of presenting author

Jiaxin Fan finished his Master by research degree and now keeps doing PhD both at the University of New South Wales. His current research topic is to discover a new method for synthesising ammonia using computational and experimental methods.



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Distribution States of Graphene in Polymer Nanocomposites for Multifunctional Properties

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Graphene has emerged as one of the promising 2D nanomaterial in polymer nanocomposites owing to its exceptional properties. The two-dimensional graphene material, when distributed appropriately in the host polymer even at low concentration can significantly alter the mass, electron and heat transfer behavior of the nanocomposites. The in-plane strong covalent bonds in graphene is accountable for the unique properties, whereas the weak van der Waals forces existing between the adjacent monolayer graphene planes are adequate to re-stack or agglomerate. Hence, the significant challenge in the production of high-performance graphene polymer nanocomposite is to alleviate the agglomeration of graphene. The agglomeration of graphene platelets can be bypassed by improving the distribution states of graphene in the matrix (1) By enhancing the dispersion and (2) By controlling the relative lattice orientation of graphene in the substrates to create an alignment. Improving the agglomerates during production will extend the benefits of graphene - mechanical, thermal, electrical and optical properties to the nanocomposite. The present study initially focuses on synthesizing stable water based graphene slurry that can be easily dispersed at high concentrations in polymer such as poly(vinyl alcohol). The exfoliated graphene nanoplatelets were 4-6 layers and the concentrated slurry exhibited stability for more than 30 days. The as prepared stable composite dispersions were then developed as foams, coatings and fiber that are further verified for piezoresistive responses with the focus to develop wearable devices (as shown in Fig. 1A). The thesis secondly focuses on developing oriented graphene based composites using the magnetic field. The high quality graphene was prepared by electrochemical exfoliation of highly oriented pyrolytic graphite and magnetically aligned in polymer matrix to explore their conductive behavior. The fundamental understanding on the structural changes of graphene dispersed in polymer solution in the presence of external magnetic field and temperature will be studied at the ANSTO using small angle neutron scattering instrument (BILBY) (as shown in Fig. 1B). The strategy to utilize neutron scattering techniques to understand the orientation of graphene will enable the optimization of electrical and thermal properties.

Bio of presenting author

Premika Govindaraj is currently a PhD student at the Swinburne University of Technology. Her research interests include 2D materials and its polymer composites with their impact in the development of smart materials.



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Connecting Structure to Membrane Performance: A Neutron Reflectometry Study of Asymmetric Polyelectrolyte Multilayers

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Micropollutants are small, stable molecules of human origin (i.e., pharmaceuticals, pesticides, plasticizers) found in aqueous environments worldwide which pose a growing risk to aquatic life and human health. The removal of these compounds from waste and drinking water poses a significant challenge. Recent studies show that porous membranes coated with asymmetric polyelectrolyte multilayers (PEMs) outperform commercial membranes for micropollutant removal. These membranes consist of a poly(styrene sulfonate) (PSS)/poly(allylamine) (PAH) support layer capped by a 'separation layer' of either PAH/poly(acrylic acid) (PAA) or PAH/Nafion. Unfortunately, the structure of these asymmetric PEMs, and thus their superior membrane performance, is poorly understood. This lack mechanistic understanding impedes the development of these asymmetric PEM separation layers.

Here we use neutron reflectometry (NR) to elucidate the multilayered structure and hydration of these asymmetric PEMs. NR reveals that the multilayers are indeed asymmetric in structure, with distinct bottom and top multilayers when air-dried and solvated. The low hydration of the top [PAH/Nafion] multilayer, together with the low water permeance of comparable [PAH/Nafion]-capped PEM membranes, demonstrate that it is a reduction in hydration that makes these separation layers denser and more selective. In contrast, the [PAH/PAA] capping multilayers are more hydrated than the support [PSS/PAH] layers, signifying that, here, densification of the separation layer occurs through a decrease in the mesh size (or effective pore size) of the top layer due to the higher charge density of the PAH/PAA couple compared to the PSS/PAH couple. The [PAH/PAA] and [PAH/Nafion] separation layers are extremely thin (~4.5 and ~7 nm, respectively), confirming that these asymmetric PEM membranes have some of the thinnest separation layers ever achieved.

Bio of presenting author

I am currently in the final weeks of my PhD at the University of New South Wales, working on understanding polymer brush behaviour through improved reflectometry analysis methods. I fill my (sadly limited) free time with houseplant-husbandry, a semi-legal distilling operation, and armies of tiny painted soldiers.



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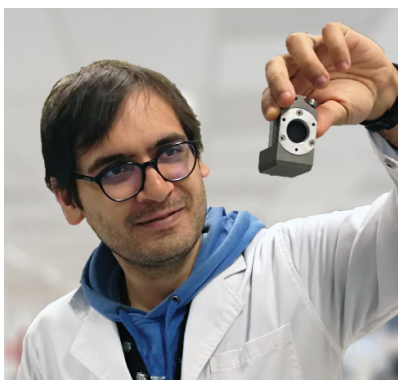
Porosity creation and evolution in the fluid-induced mineral replacement of calcite by gypsum: A SANS and USANS study

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Fluid-induced mineral replacement reactions are ubiquitous in natural environments and are important to geological and engineering processes. In these reactions, a primary mineral is replaced by a product mineral via a coupled dissolution-reprecipitation (CDR) mechanism. The dissolution of the primary mineral is spatially and temporally coupled with the precipitation of the product mineral, so that the precipitating product mineral occupies the space created by the dissolving primary mineral. This coupling leads to the preservation of the external dimension of the primary mineral into the product mineral. During the replacement reactions, porosity is created in the secondary mineral, contributing to enhanced permeability which is crucial for continued replacement in the core of the partially replaced grain. These reaction-induced pores are very complex and can evolve with time, yet the mechanism is poorly understood. Here, we study the replacement of calcite (CaCO_3) by gypsum ($\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$) to understand porosity creation during this process and evolution of the mineral's structure after the replacement reaction. This replacement reaction has important implications in groundwater reservoirs, CO_2 sequestration, cultural heritage preservation, acid mine drainage (AMD) remediation, and cement production. Samples reacted at various stages were measured by USANS/SANS, ultra-high-resolution electron microscopy (UHR-SEM) and X-ray micro computed tomography (X- μ CT). Results showed pores are created in gypsum with a wide size range from nano to micrometer; most pores are open while those below ~ 30 nm are mainly closed. After complete replacement, porosity coarsening occurred over 12 months' time, due to the Ostwald ripening mechanism; as a consequence, gypsum grains evolved to a dense gypsum layer at the outer shell and micro voids in the core.

Bio of presenting author

I did my master's degree in electrochemistry at Sakarya University, Turkey. I am currently a PhD candidate at Murdoch University under the supervision of Assoc. Prof. Fang Xia (Murdoch University) and Dr. Jitendra Mata (ANSTO), investigating the dynamics of reaction-induced porosity in minerals. In my spare time, I enjoy hiking and playing guitar.



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Influence of cladding material and grinding on the residual stress of laser clad tram rail components using Neutron Diffraction

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The successful operation of Australia's light railway networks is reliant upon the advancement of maintenance strategies to combat the increasing rate of wear and fatigue. Damages such as cracking, spalling and plastic deformation occur as

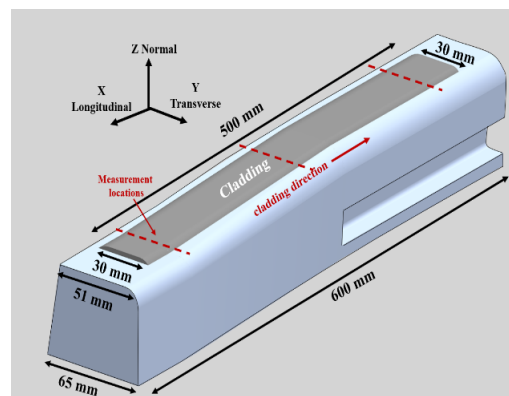


Fig. 1. Schematic of laser clad tram rail

a result of severe operation conditions due to a heightening demand for passenger transport. This requires significant government investment to finance the continuous repair and replacement of aging tramrail infrastructure. Low carbon, low alloy steel grades are characteristic of light rail and further reduce the resistance to wear and damage due to lower mechanical properties.

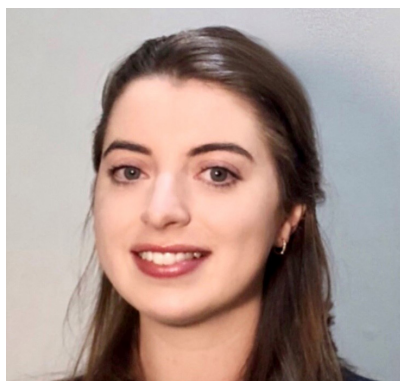
To meet the ever-increasing maintenance needs, laser cladding may be applied to worn components

to regenerate the profile or deposit a coating that imparts superior tribological properties. This is achieved by metallurgically bonding a metallic alloy at the rail surface using a high energy laser. Whilst cladding offers several advantages over standard welding repairs, thermal inputs result in heat affected regions, phase transformations and solidification shrinkage. This may introduce large tensile stresses that promote fatigue related failures.

Accurate measurement of the residual stress is essential in the development of a cladding strategy as fatigue behavior is governed by the combined effect of internal residual stress and wheel-rail contact stress. Laser cladding of three alloys, a martensitic stainless steel, Stellite 6 and Stellite 21 has been undertaken on sections of a low carbon straight tram blade (Fig 1). The triaxial internal stress distribution has been assessed within the cladding, HAZ and substrate before and after grinding, a standard finishing procedure to achieve a flat running surface that locally alters the stress state. Non-destructive neutron diffraction measurements were carried out on the Kowari strain scanner at ANSTO to experimentally obtain accurate strain data which will provide information on the rail fatigue performance. Outcomes from this investigation have been correlated to the microstructure and hardness to determine the parameters to achieve high quality depositions. This will contribute to the optimization of laser cladding repairs on tram rail substrates and understanding the stress generation after cladding low rail grades with ferritic and cobalt-chromium based alloys.

Bio of presenting author

I completed my Bachelor of Materials Engineering at Monash University where I am currently undertaking my PhD on laser cladding railway components in the Mechanical Engineering Department. In my free time I enjoy cooking and playing the piano.



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The synthesis of 19F-13C labelled aromatic amino acid probes for use in NMR spectroscopy

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19F-13C aromatic amino acid probes have recently become compounds of interest in NMR investigations of large biomolecular systems. Their use in the development and validation of 19F-13C TROSY (transverse relaxation-optimised spectroscopy) by Boeszoermerenyi et. al. provided a background-free method for probing biomolecular structure, function and dynamics.1 19F-13C TROSY is a two-dimensional (2D) experiment that harnesses the NMR-favourable properties of 19F (i.e. high gyromagnetic ratio, large chemical shift range, 100% natural abundance, and the absence of 19F in native biological systems) to observe narrow 13CF resonances and, provide high spectral resolution.1, 2 Boeszoermerenyi et. al. was able to successfully synthesise and incorporate 3-5-13C2-3-fluoro-L-Tyrosine (3-19F Tyr) into a range of biomolecules (ranging from 7-kDa to 180-kDa) and produce spectra with high sensitivity and excellent resolution (Fig. 1). Consequently, it is apparent that 19F-13C TROSY has further applications in the study of a broad range of dynamic processes such as weak binding, conformational exchange and protein folding.1, 3, 4

In their initial publication, Boeszoermerenyi et. al. proposed the synthesis of 19F-13C aromatic amino acid probes from the corresponding 13C-labelled aromatic amino acid precursors.1 As such, despite its utility in the study of large biomolecular systems, the uptake of 19F-13C TROSY as a routine NMR experiment is limited by the costliness of the starting precursors. To address this hurdle, we proposed a de novo synthetic route for building the desired 19F-13C probes from the corresponding 13C-labelled acetone.5 In addition to facilitating the synthesis of the required probes via an accessible precursor, this alternate synthetic route enables the synthesis of a variety of isotopomers which could also expand the scope of these probes beyond their use in 19F-13C TROSY.

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Bio of presenting author

Anitha Kopinathan completed her Bachelor of Medicinal Chemistry degree at Monash University in 2010, and spent the next two years working as a Research Scientist for the Centre for Drug Candidate Optimisation (CDCO) at the Monash Institute of Pharmaceutical Science (MIPS). She returned to Monash University in 2012 to complete her Honours degree and PhD in Medicinal Chemistry and Pharmacology, where her research focused on the synthesis and pharmacological evaluation of multivalent ligands targeting the dopamine D2 receptor. Following her PhD, Anitha worked as an Experimental Scientist at the CSIRO (Biomedical Manufacturing, Clayton) before taking up a Postdoctoral Research Fellowship (Medicinal Chemistry) with the ARC Centre for Fragment-Based Design in 2019. In 2020, Anitha was the recipient of an AINSE ECRG and has interests in fragment-based drug design and the synthesis of chemical probes for the investigation of proteins of interest.



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Stabilizing spinel structured lithium-ion battery electrode materials by site-selective doping

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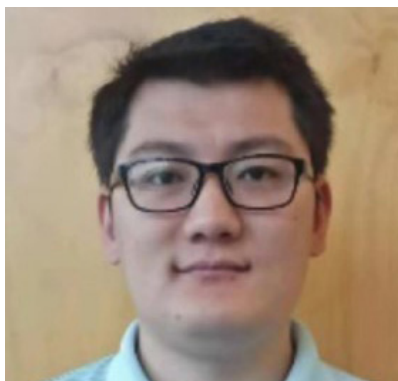
The increasing requirements of rapidly developing technologies have stimulated the development of next-generation high-performance lithium-ion batteries (LIBs). The limited energy density, of around 500 Wh kg⁻¹, of the LiCoO₂ electrode in current commercial LIBs makes them less competitive over other energy storage systems. Thus, worldwide research efforts have targeted the exploration of high-energy-density electrodes. Spinel structured LiNi_{0.5}Mn_{1.5}O₄ (LNMO) is one of the most promising candidate materials to replace LiCoO₂, due to its high operating voltage of 4.7 V vs. Li, high energy density of up to 650 Wh kg⁻¹, low fabrication cost, and low environmental impact. However, the short cycle life of LNMO caused by severe capacity decay during cycling limits its wider application and further commercialization.

Our team proposed a site-selective doping strategy to enhance the structural stability of the spinel LNMO and achieved long battery life. We considered the similar ionic radii of Mg ions at tetrahedral (8a) and octahedral (16c) crystallographic sites within LNMO with $Fd\bar{3}m$ space group symmetry (0.57 and 0.72 Å, respectively), and opted to selectively dope Mg ions onto both these sites through a facile solid-state reaction. The addition of Mg ions at such sites significantly prohibits the partially-irreversible two-phase behavior of LNMO, mitigates against the dissolution of transition metals, thus preventing the formation of the undesirable rock-salt phase and reducing the Jahn-Teller distortion and voltage polarization, consequently offering the extraordinary structure stability and cycling performance to LNMO.

This work pioneers an atomic-doping engineering strategy for the modification of electrode performance that may be applied more generally in battery research, where dopants may be used strategically to address specific electrode issues. Additionally, these findings will also facilitate the development of high-energy-density electrode materials that accelerate the commercialization of next-generation LIBs.

Bio of presenting author

I received my Bachelor's degree from Shandong University in 2014 and Master's degree from Tsinghua University in 2017. Currently I am a Ph.D. candidate at the Institute for Superconducting and Electronic Materials (ISEM), University of Wollongong, Australia. My research focuses on the high-voltage cathode materials and their mechanistic behavior in lithium-ion batteries.



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In situ neutron diffraction on U_3Si_2 corrosion experiment

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High thermal conductivity and high uranium density make U_3Si_2 a promising light water reactor fuel material, which enables a safer operation mode in terms of lower centerline temperature and the usage of more oxidation resistant cladding materials. Following the pioneer work of (Wood et al., 2018) on the thermogravimetric study of U_3Si_2 under flowing steam and elevated temperatures, we present here an in situ neutron diffraction study of U_3Si_2 under deuterated steam D_2O and the same temperature ranges. A series of pellet samples were fabricated at Los Alamos while a special sample holder with steam flow was designed and realized at ACNS.

As a preliminary result, we found that U_3Si_2 underwent mild hydrogen uptake at prolonged temperature holding at 350 °C and significant amount of hydride phase was observed from 375 °C above, after which UO_2 and an unidentified phase appeared from 400 °C with the hydride phase totally disappearing. By a series of Rietveld refinements, we propose that the hydrogen atom can be found in one of the $\text{U}_3\text{-Si}_1$ tetrahedron vacancies in the hydride phase, in contrast to the U_4 tetrahedron position proposed by (Mašková et al., 2017).

Reference

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Bio of presenting author

After finished my PhD at the University of Sydney by the end of 2020, I joined the nuclear engineering team at UNSW. My PhD was about in situ neutron diffraction, X-ray absorption spectroscopy and first principles calculation on battery materials. Currently my research interest lies in in situ neutron diffraction of nuclear fuel materials. Before coming to Australia, I did my Master's degree on electron microscopy characterization of battery materials at Central South University.



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Nanoparticles and Surfactants: How they live, and how they dry

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The drying mechanism of surfactant solutions and nanoparticle suspensions is important for their applications in coatings and paints, and is decidedly non-trivial. In addition to factors such as contact line pinning, surface tension, Marangoni forces, etc. that come into play for deposition, the changing concentration due to drying is complicated by the self-assembly of surfactant molecules into either micelles or liquid crystal phases. This work aimed to examine how the formation of these self-assembled phases affects the drying process of systems containing both surfactant and nanoparticles.

Phases were designed with 0-60 % w/w dodecyltrimethylammonium bromide (DTAB, a cationic surfactant) and 0-5 % w/w 10 nm (diameter) silica nanoparticles. Larger concentrations effectively represented structures that were drier. Structural analysis was undertaken using small-angle neutron scattering (SANS), ultra-small-angle neutron scattering (USANS), and polarising light microscopy (PLM). Viscosity measurements were taken using a benchtop rheometer with a cone-and-plate set-up.

Silica nanoparticles were found to flocculate in these systems, though the size of these flocs decreased as the concentration of DTAB was increased. In turn, this decreased the opacity of the systems. Additionally, the viscosity of these systems increased as the concentration of either component was increased.

When droplets of silica solution were dried and examined using PLM, it was found that silica particles dried into large structures in the centre of the droplet. When DTAB was present, the far more birefringent surfactant crystals were found beyond the silica structures, and were also apparently incorporated into the silica structure. At higher concentrations of DTAB, the silica structures were disrupted, likely as a consequence of the smaller flocs in solution. This caused a more homogeneous drying process compared to the samples with silica, but with a decreased birefringence compared to a silica-free system. This latter effect was likely because the smaller silica flocculates could act as defects in the wider surfactant crystal structure, weakening the long-range order and birefringence.

Bio of presenting author

I completed my Honours and PhD research at Monash University, and have recently begun a Postdoctoral Research Associate position working with Prof Greg Warr at The University of Sydney. Research interests include small-angle scattering and the self-assembly of surfactant systems. My pronouns are he/him/his.



**Joshua
Marlow**

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Novel Processing of Pyrite Ore to Produce Battery Grade Cobalt and Sulfur

With the Australian resource sector being responsible for more export income than all other national industries combined (Constable, 2019), the need to continuously improve productivity in mineral ore processing is essential. Reducing the cost of raw mineral processing and production of commercial grade compounds, and appropriately scaling these technologies to industrial levels, are key optimizations to this sector to enable Australian exports to remain competitive in the global mining industry. The presence of large cobalt-pyrite ore deposits in Australia has created a demand for the extraction of valuable cobalt and sulfur. Reducing the cost of liberating and converting these elements into commercially applicable compounds, such as cobalt sulphate for such applications as cathodes in lithium-ion batteries, is of interest. Mineral extraction via acidic leaching and roasting/sintering of solid ores are commonly used industrial techniques but often require multiple stages of mineral decomposition before commercial-grade compounds are produced. A novel thermal decomposition process of pyrite ores has been proposed. This is a process of extracting cobalt and sulfur from pyritic feedstocks, able to produce battery grade compounds while extracting additional valuable resources (such as gold) sometimes found in high gangue ores. The new technique must be optimized, and is part of a research initiative using custom small-scale furnaces provided by 'ANERGY'. Previous work with this technique has involved characterizing ore grain sizes and how this influences their interactions with conditions such as carrier gas and other particles in heating zones. With goals of reducing processing costs and maximizing resource yields in mind, the first aim of this project is to characterize furnace conditions to achieve optimal thermal decomposition of pyritic ore to produce the desired compounds derived from cobalt and sulfur and extract other potential valuable resources. Conditions such as ore particle size, mixing regime for material phases, carrier gas flow and heating zones/timing will be explored to better characterize the decomposition process. Using the preliminary work from 'Cobalt Blue', fine ore particle sizes ($\sim 300\text{ }\mu\text{m}$) are required in this system to effectively prevent the loss of material in the carrier gas while maximizing surface reaction area for liberation of gaseous sulfur compounds. This work will be supported by Computational Fluid Dynamics (CFD) modelling to more effectively optimize the aforementioned conditions. The second aim of this project involves using the data retrieved from the laboratory scale reaction mechanisms under varying conditions to better understand the potential of upscaling this thermal decomposition process, ultimately aiming for a means of reaching an industrial/commercial scale. Samples will be characterized using neutron and X-ray powder diffraction using the resources available at ANSTO, UNSW and the Australian Synchrotron. These analytical techniques will be applied to elucidate structures and phase composition of materials produced within the furnace under various conditions using quantitative phase analysis (QPA). With the optimization of this novel technique, the more efficient extraction and production of battery grade cobalt and sulfur will be useful to the expanding electric automotive market fostering further investment into industries concerned with processing of pyritic ore deposits.

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Bio of presenting author

Hamish commenced the MIR program in T2 (2020) with Cobalt Blue and is working with Ass Prof Suzanne Neville (UNSW), Prof Vanessa Peterson (ANSTO) and Dr Andrew Tong (CoB). Hamish has a chemistry background from the UOW focusing mainly on atmospheric, analytical and material chemistry. He loves astronomy, space, and theoretical physics. Most importantly, Hamish is a huge gaming nerd (mostly shooters), and a Minecraft professional.



**Hamish
McDougall**

University of
New South Wales

Academic Level
Other

ACNS Co-supervisor
Vanessa Peterson

Controlling the precipitation sequence in Al-Cu-Li alloys using Sc and Zr additions

Al-Cu-Li alloys are extensively used in modern aircrafts as they exhibit an excellent balance between weight and strength. However, the constant development of new materials challenges the competitiveness of these alloys, leading to continuous research to improve their mechanical properties. Adding Scandium (Sc) and Zirconium (Zr) to Al-alloys is known to enhance the material's strength, with a limited impact on ductility. This is due to nano-size $Al_3(Sc,Zr)$ dispersoids that form with a core/shell morphology. The interaction between these dispersoids and the Cu and Li containing precipitates is currently unknown.

In the present work, model alloys were designed to explore the addition of Sc and Zr in an Al-Cu-Li alloy. Three alloys were cast: Al-Sc-Zr, Al-Cu-Li-Zr and Al-Cu-Li-Sc-Zr. These alloys were subsequently examined in selected tempers, partially including pre-stretch prior to artificial ageing. The precipitation behaviour was characterised with Transmission Electron Microscopy (TEM) and Differential Scanning Calorimetry (DSC). It was found that Sc significantly changes the ratio between the volume fraction of the θ' , θ'' and T1 phases. Consequently, the balance between strength and ductility was affected. It is suggested that this might be utilised to adjust the mechanical properties tailored for the alloy's application.

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**Katrin
Mester**

Deakin University

Academic Level
ECR

ACNS Co-supervisor
Kathleen Wood

Bio of presenting author

I have done my bachelor's and master's degree of material's engineering at RWTH Aachen University near my hometown Cologne in Germany. I have then started a PhD at the Institute for Frontier Materials at Deakin University in Victoria, where I focused on precipitation in aerospace alloys.



Flexibility of Lipid Bilayer Membranes in Ionic Liquids

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Ionic liquids (ILs) are a novel class of solvents with ultra-low vapour pressure and tunable liquid properties. Protic ILs are particularly effective solvents for self-assembly of surfactants and lipids into micelles, vesicles, liquid crystals and microemulsions.[1] This is exemplified by alkylammonium ILs, which are also cheap, easily prepared and can be readily deuterated. Over the past decade, much is learnt about the nanostructure of many alkylammonium ILs,[2] but virtually nothing is known about solvent nanostructure affects the dynamics of amphiphile aggregates. In this work, we aim to reveal the effect of solvent nanostructure on flexibility of lipid bilayers. We employed neutron spin echo spectroscopy (NSE) on IN15 at the ILL to probe the mesoscopic undulations of Egg-PC membranes (1 wt% as vesicle dispersions) in two ILs, ethylammonium and ethanolammonium formate, and their mixtures with water. For the first time, IN15 was configured to perform dynamic measurements up to 1000 ns.[3] By combining NSE with SANS and DLS, we observed the lipid bilayers to be potentially an order of magnitude softer in ILs without significant changes in their thickness. This surprising finding cannot be fully accounted for with available theories and confirms that the effect of solvent should not be overlooked in future. This work has the potential to add a new dimension for tuning and designing membrane behaviour, as well as exploring the idea of potential lifeforms in non-aqueous environments.

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Bio of presenting author

I did my Honours research at the University of Sydney and I am now a PhD candidate within the same research group. My research is centered on ionic liquids but the topic I cover is quite broad, ranging from fundamental structural study of liquid system, to self-assembly and soft matters. I play badminton and like to travel (pre-COVID hobby).



**Shurui
Miao**

The University of
Sydney

Academic Level
PhD (3rd year)

ACNS Co-supervisor
Katy Wood

Use of a Miniature Diamond-anvil Cell in a Joint X-ray and Neutron High-pressure Study on Copper Sulfate Pentahydrate

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Single-crystal X-ray and neutron diffraction data are usually collected using separate samples. This is a disadvantage when the sample is studied at high pressure because it is very difficult to achieve exactly the same pressure in two separate experiments, a particular problem if the neutron data are collected using Laue methods where absolute values of the unit-cell dimensions cannot be measured.

Diffraction data have been collected using precisely the same sample of copper (II) sulfate pentahydrate, using a conventional laboratory diffractometer and source for the X-ray measurements and the KOALA single-crystal Laue diffractometer at the ANSTO facility for the neutron measurements. The sample, of dimensions $0.40 \times 0.22 \times 0.20$ mm³ and held at a pressure of 0.71 GPa, was contained in a miniature Merrill-Bassett diamond-anvil cell. The highly penetrating diffracted neutron beams passed through the metal body of the miniature cell to yield data suitable for structure refinement, compensating for the low completeness of the X-ray measurements, only 24% on account of the triclinic symmetry of the sample and the shading of reciprocal space by the cell. The two data sets were combined in a single 'X-N' structure refinement in which all atoms, including hydrogen atoms, were refined with anisotropic displacement parameters. The precision of the structural parameters was improved by a factor of up to 50% in the X-N refinement compared to refinements using the X-ray or neutron data separately.

Bio of presenting author

I did my Master Degree in Pharmacy in Italy, at the Università di Modena e Reggio Emilia. I am in the final year of my PhD in Crystallography that is affiliated jointly between the University of Edinburgh and the Australian Centre for Neutron Scattering at the Australian Nuclear Science and Technology Organisation (ANSTO) near Sydney. My research has focused on the development of single-crystal and powder diffraction techniques at large scale facilities in order to study the phase behaviour of molecular materials at extreme conditions, in particular, high pressure.

In my spare time I love reading books and walking in the countryside.



**Giulia
Novelli**

University of
Edinburgh

Academic Level
PhD (3rd year)

ACNS Co-supervisors
Garry J. McIntyre &
Helen E. Maynard-
Casely

Investigating the anharmonic collapse of phonon dispersions in SnSe through inelastic neutron scattering

Thermoelectric materials offer an alternative and clean source of electrical energy to modern sources as a direct conversion of thermal energy. These materials operate via the Seebeck effect in which a temperature gradient produces a voltage difference between substances. Appropriate materials for use in thermoelectric devices are those with very low thermal conductivity and a high thermoelectric power factor.

Devices such as Peltier cooling thermoelectrics have the benefit over standard vapor compression refrigeration as they have no moving parts, no refrigerant fluids, long lifetime, and are not as restricted by shape or size.

The orthorhombic Tin Selenide (SnSe) presents itself as a promising thermoelectric material as it has an ultralow thermal conductivity due to a high anharmonicity and high thermoelectric power factor. SnSe also exhibits a structural transition from the Pnma group to the Cmcm group at a critical temperature of $T_C = 800$ K which further increases the anharmonicity of the acoustic and optic branches [1].

This work aims to study and map phonon dispersions of SnSe before and after the structural transition to further our understanding of the underlying atomistic process in anharmonic phonon propagation and, further, to relate this to the thermal conductivity of materials.

Inelastic neutron scattering on a single crystal of SnSe in the Pnma state has been performed at room temperature using Taipan to successfully locate some of the acoustic phonon branches in the [0KL] plane. Time of flight inelastic scattering data from Pelican has also been taken on a SnSe powder sample which has indicated that optic phonon branches exist below 20meV.

Further experimentation will be performed at different temperatures to map the phonon dispersions at higher temperatures, particularly after 800 K where the structure will change to Cmcm symmetry. Here, we expect to see a softening of the phonon branches as the structure begins to change [1].

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Bio of presenting author

For the past 3 years I have been doing a bachelor of science at the university of Wollongong majoring in physics and I will be commencing my honours year doing research at ANSTO this year. My research project will be based on measuring phonon dispersions using inelastic neutron scattering and I am particularly interested in strange quantum effects.



**Kyle
Portwin**

University of
Wollongong

Academic Level
Honours student

ACNS Co-supervisor
Kirrily Rule

Catalytic Nucleophilic Alkylation of Benzene + image

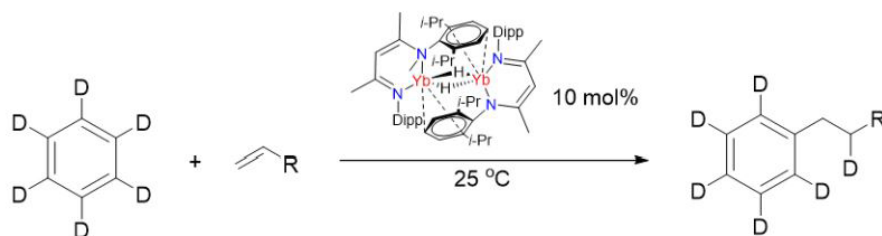
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Alkylation of aromatic systems an important transformation both academically and industrially. This is typically achieved via an electrophilic substitution (Friedel-Crafts) mechanism, however, this reaction suffers significant drawbacks such as polyalkylation and poor selectivity to linear alkylated products. These limitations may be avoided by utilizing an alternate mechanistic pathway, direct nucleophilic substitution. Herein, I will discuss the successful synthesis of a low-coordinate ytterbium(II) hydride, $[(\text{BDIDipp})\text{YbH}]_2$ ($\text{BDI} = \text{CH}[\text{C}(\text{CH}_3)\text{NDipp}]_2$, $\text{Dipp} = 2,6\text{-diisopropylphenyl}$). Reactivity studies demonstrate the ytterbium(II) hydride can sequester the unactivated alkenes, ethene and propene, to generate the corresponding primary Yb(II) n -alkyls, $[(\text{BDIDipp})\text{YbR}]_2$ ($\text{R} = \text{Et}$ or Pr). Both were found to facilitate the alkylation of either protio or deuterobenzene at room temperature via a nucleophilic $\text{S}_{\text{N}}2$ -like substitution of the aromatic C-H/D bond, a reaction mechanism which is supported by Density Functional Theory (DFT) calculations. Regeneration of $[(\text{BDIDipp})\text{YbH}]_2$ allows for further reactivity with either ethene or propene, thus mediating the catalytic alkylation of benzene.



Scheme 1. Catalytic nucleophilic alkylation of benzene

Bio of presenting author

I did my Honours research at Victoria University of Wellington and have just begun my PhD at the same institution, with my research topic for both focusing on Arene C-H Activation by Lanthanide Complexes. Main hobbies include swimming and watersports.



**Georgia
Richardson**

Victoria University
of Wellington

Academic Level
PhD (1st year)

ACNS Co-supervisor
Alison Edwards

Untangling protein- G-quadruplex interactions in heterochromatin formation

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*lead presenter

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Each human nucleus contains a vast amount of genetic information. A total of six billion base-pairs equalling two meters in length fit into a space just six microns across. The way in which DNA is able to organise itself in this minuscule space is through the formation of the complex architecture of chromatin, a nucleoprotein complex.

Chromatin consists of histone octamers encircled by DNA to form nucleosomes. The variation in histone type and the post-translational modifications deposited upon them are what dictate the form of chromatin. Heterochromatin is the compact form of chromatin, required to protect certain regions of the genome, and requires the recruitment and maintenance of Heterochromatin Protein 1a (HP1a).

The current histone code relies on the fact that HP1a is recruited to and binds chromatin through its interaction with trimethylated histone H3 on lysine 9 (H3K9me3) by its chromodomain. However, this interaction is low affinity, and ignores evidence that the hinge of HP1a, as well as a contribution of RNA are required to target and retain HP1a on heterochromatin.

My work has shown that HP1a binds with high affinity to DNA and RNA folded into G-quadruplexes (G4s), a non-canonical form of nucleic acid formed by four guanine nucleobases bound in a tetrad, stacked to form a quadruplex. I found that HP1a binds G4s of parallel topology, while not preferring G4s of an anti-parallel topology. Given this distinct selectivity of HP1a, I now seek to scrutinise HP1a structure, how it interacts with G4s, and examine how the HP1a-G4 interaction regulates its function in heterochromatin. It is hoped that this work will highlight the long-ignored role of non-canonical nucleic acids in our genomes, and how HP1a facilitates this through formation of protective heterochromatin.

Changing the paradigm of heterochromatin formation will ultimately underpin development of new and innovative technologies in cancer treatment, through providing insights into novel DNA binding chemotherapies by developing druggable targets of unique G4 structures.

Bio of presenting author

Having completed my Master of Science degree at Massey University in Palmerston North (NZ), I have now begun my journey towards a PhD in Biochemistry in the same lab, tweezing apart weird protein-nucleic acid interactions. Out of the lab, I'm either DIYing or attempting to mountain bike.



Ruby
Roach

Massey University

Academic Level
PhD (2nd year)

ACNS Co-supervisor
Katy Wood

Unravelling specific ion effects: A neutron reflectometry study of thermoresponsive polymer brushes in complex environments

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Specific ion effects are ubiquitous in nature and industry and relate to any phenomena which depend on the identity of ions present in a system, not merely their valence or concentration. One subset of specific ion effects is the Hofmeister series, which orders ions on their ability to either stabilise (salting-in ions) or destabilise (salting-out ions) macromolecules in a system. [1] In recent years, thermoresponsive polymer brushes have been used as exemplar systems to study specific ion effects.[2] Thermoresponsive polymer brushes, such as poly(oligo(ethylene glycol) methacrylate) (POEGMA) and poly(N-isopropylacrylamide) (PNIPAM) consist of a dense array of surface tethered polymers that undergo a phase transition from well to poorly solvated over a given temperature range; establishing an interface with switchable physicochemical properties.

A paucity currently exists in understanding the influence of mixed and non-aqueous electrolytes on the behaviour of polymer brushes. To date, no all-inclusive theory regarding specific ion effects exists, however, as natural environments are comprised of complex electrolytes, understanding the interplay of different ions in various solvents is imperative for real world applications. The thermoresponse of a POEGMA statistical copolymer brush was monitored in a variety of mixed aqueous electrolytes,[3] which unveiled a non-monotonic concentration-dependent influence of the two anions on the thermoresponse of the brush. The influence of non-aqueous solvents (dimethyl sulfoxide, formamide and propylene carbonate) on the thermoresponse of a PNIPAM brush has also been probed in the presence of various ions, where particular solvents induce a Hofmeister series reversal. Neutron reflectometry (PLATYPUS) is employed across these studies to understand the subtle differences in polymer brush conformation, and thus the myriad interactions between the solvent, solute and substrate in an attempt to elucidate the dominate drivers behind ion specificity.

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Bio of presenting author

I completed a BSc (Hons)/(Chemistry)/BMath at the University of Newcastle in 2019, and I am currently in my second year of my PhD at the University of Newcastle. In my research, I use thermoresponsive polymer brushes as exemplar systems to investigate specific ion effects in complex environments.



**Hayden
Robertson**

University of
Newcastle

Academic Level
PhD (2nd year)

ACNS Co-supervisor
Andrew Nelson

Effect of the geometrical confinement on the water and lipids dynamic in biomimetic lipidic cubic phases.

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Lipidic mesophases are complex structures naturally formed by hydrated lipids and employed for a range of application that span from membrane protein crystallization^{1,2,3} to drug delivery and biosensors⁴. Understanding the dynamic of water and lipids in these matrices is of general interest in the field⁵ and extremely

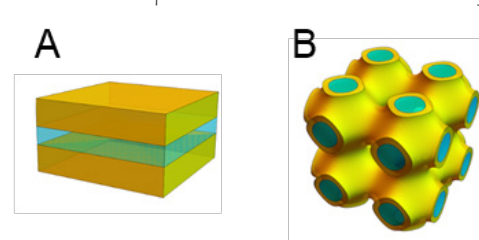


Figure: Example of lipidic mesophases: A) Lamellar B) Cubic

important in developing new drug formulations, as well as in developing new tools for biosensors and membrane protein crystallization.

We recently demonstrated that lipidic cubic phases with extremely small water channels (<1 nm) are efficient matrices to confine water and to avoid freezing at sub-zero temperature.⁶

We are currently employing quasi-elastic neutron scattering (QENS) measurements on Emu and Pelican to monitor the dynamic of lipids and water in different geometries and with different degrees of confinement.

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Bio of presenting author

I obtained my PhD from University of Zurich. Between 2017 and 2019 I did a postdoc in ETH Zurich. Currently, I am a SNF postdoctoral fellow at the University of Sydney. I am recently been awarded a AINSE ECR grant. My research is focused on the development of lipidic mesophases for biochemical studies.



Livia
Salvati Manni

University of Sydney

Academic Level
ECR

ACNS Co-supervisor
Alice Klapproth

Scaling behaviour of the skyrmions in Cu₂OSeO₃ single crystals from small angle neutron scattering

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A skyrmion is a topological stable particle-like object comparable to a spin vortex at the nanometre scale. It consists of an about 50 nm large spin rotation and its spin winding number is quantised. Skyrmions emerge in chiral crystals upon competing symmetric exchange and asymmetric Dzyaloshinskii-Moriya (DM) interactions and typically form two dimensional hexagonal lattices perpendicular to an applied magnetic field. Its dynamics has links to flux line vortices as in high-temperature superconductors [1-2].

Cu₂OSeO₃ is a unique case of a multiferroic material where the skyrmion dynamics could be controlled through the application of an external electric field, which could enable energy-efficient data storage and data processing devices, and testing fundamental theories also related to the Higgs Boson whose theoretical description has similarities to skyrmions [3].

The technological applications depend on the stabilisation of the skyrmion phase up to room temperature. While some materials host skyrmion lattices above room temperature [3], Cu₂OSeO₃ is the only insulating skyrmion material discovered so far, which orders magnetically below 58 K. Noticeably, the appearance of two different skyrmion phases have been reported along the magnetic phase diagram of Cu₂OSeO₃ when the sample is aligned with its <100> or <110> crystallographic axes parallel to the incoming neutron beam and performing Zero Field Cooling (ZFC) or Field Cooling (FC) across the high-temperature skyrmion phase. However, the stabilisation processes of these two phases and their thermodynamic connection are still under debate [4-6]. We have used small angle neutron scattering and Lorentz transmission electron microscopy [7] to study the scaling behaviour of helical phase and the magnetic skyrmion lattices, i.e. the systematic change of their distances in single crystals of Cu₂OSeO₃ in order to gain insight on the balance between the different competing magnetic exchange interactions.

Therefore, we have examined the field, temperature, and sample alignment dependence of the scaling behaviour of skyrmions as an order parameter for the emergence of the two skyrmion phases. The obtained data provide valuable information on the formation mechanism of the skyrmions and their stability range. This is an important step towards the understanding of the manipulation of skyrmions, which is required for technological applications.

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Bio of presenting author

I did my master's research under the supervision of Prof. B. Keimer at the Max Planck Institute for Solid State Research in Germany. Currently, I conduct my PhD studies under the supervision of A/Prof. C. Ulrich at the University of New South Wales. In both institutions I have applied spectroscopic techniques to investigate Strongly Correlated Electron Systems. I play chess and soccer in my spare time.



**Jorge A.
Sauceda
Flores**

University of
New South Wales

Academic Level
PhD (3rd year)

ACNS Co-supervisor
Elliot Gilbert

Plasma Treatment: A Systematic Approach to Probe CelluloseMucin Interactions in Thunderstorm Asthma

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3University of Sydney, Sydney, Australia

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Plasma, most commonly known as fourth state of matter, is a mixture of myriad of reactive chemical species that are electrically generated by splitting gaseous molecules. The wellknown natural phenomenon of lightning and thunderstorm generates reactive oxygen and nitrogen species (RONS) that are dissolved in the atmospheric moisture altering its chemical properties creating so-called plasma activated water (PAW). The air-plasma (AP) and PAW are proposed to significantly affect the surface-chemistry of airborne biological microparticles such as grass pollen grains. Thunderstorm-borne pollens have been linked to the development of epidemic thunderstorm asthma (ETSA), however, the fundamental molecular cause and mechanism of ETSA is poorly understood. In this research, we have mimicked thunderstorm conditions by generating air-plasma and PAW, and associated molecular components such as cellulose (pollen coat) and mucin (tracheal mucosa) and elucidated the biointerfacial interactions by employing advanced interface-sensitive techniques including quartz-crystal microbalance with dissipation (QCM-D) and neutron reflectometry (NR).

Our results indicate that both AP and PAW significantly alter the surface chemistry of cellulose and its subsequent interactions with mucin. In particular, the adsorption of mucin on PAW-treated surface increases with the increase in treatment time of cellulose, which implies a role for wettability of cellulose in determining mucin adsorption and therefore stronger downstream immune reactions. Additionally, we prepared PAW via dielectric barrier discharge (DBD) method under different plasma conditions (frequency, voltage) to decipher the variability of mucin interactions with different PAW-treated cellulose surfaces and observed that it results in stronger initial interactions. Furthermore, we performed neutron reflectometry to probe the structural alterations in mucin on different plasma-treated cellulose surfaces and examined the different layer thickness and volume fraction profiles, which implies the different arrangement of mucin on AP-treated and PAW-treated representative cellulose surfaces. This systematic approach to solving fundamental yet critical cellulosemucin interactions not only presents an ideal model system for efficient characterization but also enables the development of better diagnostics and therapeutic interventions for thunderstorm asthma.

Bio of presenting author

I am studying PhD at the University of New South Wales, with my research topic on particle formation and characterization of biointerfacial interactions in the development of thunderstorm asthma. I am an avid fan of cricket and play cricket in my spare time.



**Arslan
Siddique**

University of
New South Wales

Academic Level
PhD (2nd year)

ACNS Co-supervisor
Andrew Nelson

Understanding the chemical/mechanical function of non-conjugated dicarboxylic acids as organic electrode materials for lithium-ion batteries

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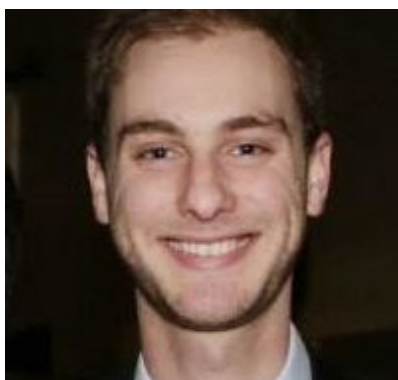
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Current commercial battery technology uses materials that are typically expensive, toxic, environmentally hazardous, and non-renewable. Organic electrode materials (OEMs) address many of these issues as they are often low-cost, non-toxic, environmentally friendly, and made from feedstock chemicals. This work focuses on a promising class of OEMs, the small, readily available, and simple, non-conjugated dicarboxylic acids as an anode in lithium half cells and rationalises the relationship between chemical/microstructure and electrochemical performance.

In particular, the electrodes microstructures are explored in depth, which is an area often overlooked in the emerging field of OEMs. SEM, XRD SANS and USANS are used to understand the microstructures of the electrodes, ultimately enabling rationalisation of some of the trends observed in the electrochemical performance. These results provide the groundwork for the rational design/selection of more promising OEM-based anode materials which may lead to the development of a wholly OEM-based lithium-ion battery.

Bio of presenting author

I did my Honours research at the University of New South Wales and am in the second year of my PhD at the University of New South Wales. My research focuses on the evaluation and characterisation of novel organic electrode materials for next generation lithium and sodium ion batteries. Between my Honours and starting my PhD I worked for the ANSTO spinoff Ceramisphere.



**Matthew
Teusner**

University of
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Academic Level
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Understanding of pepsin induced protein coagulation in skim milk

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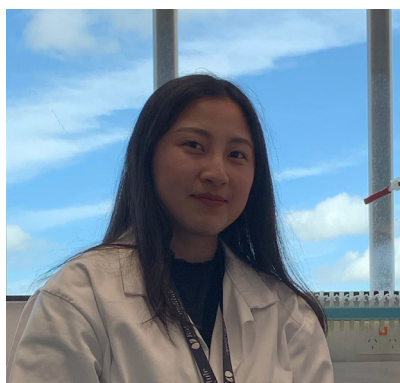
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In milk and dairy product digestion, coagulation of casein micelles occurs and plays a key role in the gastric transit of proteins. This coagulation is induced by specific hydrolysis of the Phe105-Met106 bond of κ -casein which is catalyzed by pepsin when $\text{pH} > 5$, and which results in destruction of the protective effect by κ -casein on the casein micelle surfaces. The mechanism and kinetics of κ -casein hydrolysis induced by pepsin and the relationship between hydrolysis and casein coagulation have not been previously reported. In this study, the effect of pH (6.7 - 5.3) and pepsin concentration (0.11 - 2.75 U/mL) on κ -casein hydrolysis and the coagulation properties of casein micelles in cows' skim milk were investigated at 37°C using reverse-phase HPLC, oscillatory rheology, and confocal laser scanning microscopy (CLSM). It was shown that the hydrolysis of κ -casein followed first-order kinetics. Increasing the pepsin concentration increased the hydrolysis rate and reduced the coagulation time. The hydrolysis rate was also pH dependent and reached a maximum at $\sim\text{pH}$ 6.0. As the decrease in pH reduces the electrostatic repulsions between para-casein micelles, the extent of κ -casein hydrolysis required for coagulation decreased markedly from 70% to 40% when pH decreased from 6.7 to 5.3.

The evolution of storage modulus (G') and the firming rate (dG'/dt) of the coagulum with hydrolysis time were strongly affected by the pH and pepsin concentration, which generally matched well with the coagulum microstructures observed by the CLSM. However, due to the syneresis of coagulum caused by small oscillatory deformation during rheological measurements, the value of G' max could not reflect the strength accurately. As a consequence, small angle scattering techniques that allow the probing of the structure of protein aggregates in situ will be required for further investigations. The structure of casein micelles and the colloidal calcium phosphate (CCP) nanocluster features will be probed by small-angle neutron scattering (SANS); the size and structures of large-scale protein coagulum on the micron scale will be probed by ultra small angle neutron scattering (USANS). In addition, as small angle X-ray scattering (SAXS) can reveal the protein inhomogeneities (2 - 3 nm) in casein micelles, it will be used to study the casein protein matrix rearrangement during coagulation.

Bio of presenting author

I am a second year PhD student at Massey University, NZ. I did my BA from Zhejiang University of Science and Technology, CN; MA from Wageningen University, NL; and an internship in the University of British Columbia, CA. I am now investigating the interactions between milk protein and digestive enzymes (pepsin), which provides fundamental knowledge for milk digestion. I have research experience in characterizing the physicochemical properties of food components using rheology, tribology, microscopic techniques, and aiming to probe the structural changes of food components during processing and digestion with neutron scattering techniques in the future.



Mengxiao
Yang

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Effect of ionic strength on the rheological and structural characteristics of thermally induced quinoa protein gels

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The effect of ionic strength on the heat-induced gelation of quinoa protein isolates (QPI) at pH 7 were investigated. The gelation behaviour and gel strength were characterised by oscillatory rheology. The microstructural characteristics of QPI solutions and gels were probed by ultra-small angle neutron scattering (USANS), small-angle X-ray and neutron scattering (SAXS, SANS), and confocal laser scanning microscopy (CLSM). This suite of techniques provided structural details covering a wide range of length scales, from tens of micron to nanometre. It was found that the gelation temperature decreased from 73 °C to 40 °C and the G^* (1 Hz) increased from ~67 Pa to ~1285 Pa with increasing the concentration of NaCl from 0 to 200 mM. A small protein particle size of ~32 Å and ~57 Å was identified within the QPI gel containing 0-200 mM NaCl from SAXS and SANS, respectively, while this size feature is diminished upon addition of CaCl₂. For all QPI samples, heat treatment promoted protein aggregation at micron scale, while the larger structural unit ($R_g \sim 170$ nm) kept intact as revealed by USANS. A similar mass fractal structure ($df=2$) was observed in the QPI gels containing 0-200 mM NaCl, while CaCl₂ addition caused the formation of large protein agglomerates ($R_g \sim 2.5$ -4.0 µm) with a more compact and denser structural organisation ($df=2.5$) inside the protein blobs. CLSM showed that the QPI gels containing CaCl₂ are prone to phase separation. Overall, this finding shows the thermal gelation behaviour of QPI can be modulated by the ion type and concentration, which is similarly observed in other globular protein systems.

Bio of presenting author

Zhi Yang obtained a PhD from University of Auckland in 2016. After that, he worked as a postdoctoral fellow in National University of Singapore, University of Auckland, and the Oak Ridge National Laboratory. He recently joined Massey University as a lecturer. His research work deals with the structure-function of food biomacromolecules like starch, dairy and plant proteins, and cellulose in gels, emulsions, and concentrated solutions. His work involves the use of small angle scattering methods (SAXS, SANS, and USANS) to investigate in-situ the effect of stressors, such as heat, high hydrostatic pressure, and shear, on biological macromolecules.



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Potential-Dependent Superlubricity of Ionic Liquids on Graphite Surface

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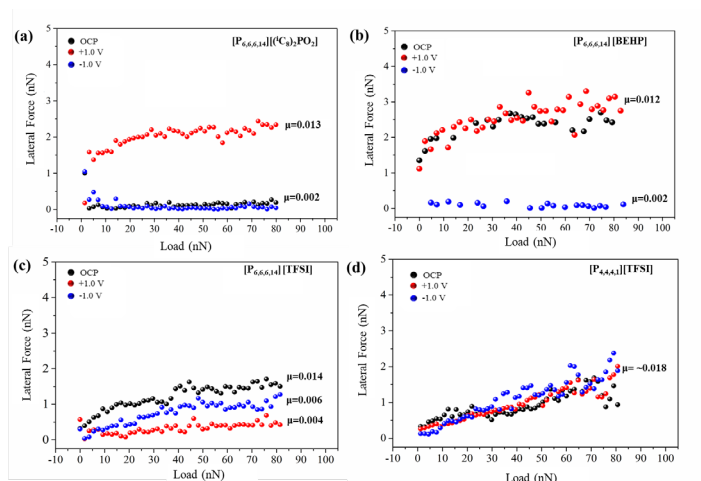
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The lubricities of four quaternary phosphonium ionic liquids, trihexyltetradecylphosphonium bis(2,4,4-trimethylpentyl)phosphinate ([P_{6,6,6,14}][(C₈)₂PO₂]), trihexyltetradecylphosphonium bis(2-ethylhexyl)phosphate ([P_{6,6,6,14}][BEHP]), trihexyltetradecylphosphonium bis(trifluoromethylsulfonyl)imide ([P_{6,6,6,14}][TFSI]) and tributylmethylphosphonium bis(trifluoromethylsulfonyl)imide ([P_{4,4,4,1}][TFSI]) were measured as a function of potential on highly oriented pyrolytic graphite (HOPG) using atomic force microscopy (AFM).

Frictions change as the compositions of the boundary layers switch from cation-enriched to anion-enriched when the potential changes from negative to positive. Superlubricity, which refers to near zero increase in friction with load, is achieved for the [P_{6,6,6,14}]⁺ cation at -1.0 V and the [TFSI]⁻ anion at +1.0 V. The lubricities of ILs are mainly influenced by three factors: the alkyl chain length, chemical composition and ion sizes.

These experiments were conducted on AFM which has a sharp tip sliding on surface, and further friction track information is hard to collect due to the tiny contact area (~8nm radius). Neutron reflectivity will provide information about the ion conformation and layer composition on surface, and how they change with surface potentials. These will help understand friction behavior.

Key words: ionic liquid; potential-dependent; superlubricity, Neutron Reflectivity



Lateral force vs. normal load of four ILs at OCP, -1.0 V and +1.0 V on HOPG: (a) [P_{6,6,6,14}][(C₈)₂PO₂], (b) [P_{6,6,6,14}][BEHP], (c) [P_{6,6,6,14}][TFSI] and (d) [P_{4,4,4,1}][TFSI].

Bio of presenting author

I got my bachelor degree from North University of China majoring Chemical Engineering at 2015, and master degree from Shanghai University majoring Polymer Chemistry at 2018. I started to the research of tribology of ionic liquids from my 2016 and now working with Prof. Rob Atkin and Dr. Hua Li at UWA.

I like guitar, badminton, snorkeling in my spare time.



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Anton Le Brun

Phonon Modes in ZrGeSe

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ZrGeSe is a quasi-two-dimensional material with fascinating topological nodal-line electronic band structure. We have investigated the phonon excitations in ZrGeSe via TAIPAN triple axis spectrometer. Both the

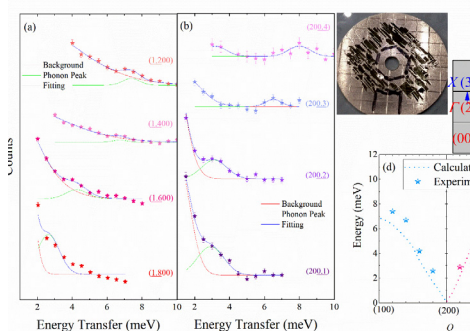


Fig 1 Acoustic phonons of I-Z zone: (a) longitudinal phonon; (b) one branch of transverse phonon. (c) The coaligned ZrGeSe single crystals on an aluminum disk, & a sketch of I-Z zone in reciprocal lattice.

longitudinal and transverse acoustic phonon dispersions have been observed along (q00) direction, which agrees well with previously calculations. Optical phonons are also observed at several Q values, which all populated between 14 and 28 meV, with gapless feature.

As an example, Fig. 1 demonstrates the energy scans at several different Q positions with 0.5 meV step on TAIPAN at 300 K. Theoretically the phonon modes will be symmetric

in (2+q00) side and (2-q00) side, however the detector presents better resolution on (2-q00) side. We thus perform the longitudinal acoustic (LA) mode energy scans in I-X zone on (2-q00) side at 300 K and chose 4 points between zone center and zone boundary, as shown in Fig. 1(a). Further, we conduct the transverse acoustic (TA) mode energy scans in (200+q) zone, with 4 different q values between zone center and zone boundary, which are shown in Fig. 2(b). After carefully fitting the experimental counts with Gaussian peaks, we obtained the LA and TA phonons propagating along (q00) direction. The experimental LA and TA phonons are summarized in Fig. 2(c) with star symbols, to compare with the DFT calculations (dash lines), in which one can see the tendency of dispersions of both phonon modes agree well from calculation to experiments, however with slightly energy soften.

We also obtained the optical phonon modes, the highest of which is ~ 25 meV.

Bio of presenting author

I am a PhD student in Institute for Superconducting and Electronic Materials, University of Wollongong, working on topological materials. I am good at single crystal growth of inorganic compounds and catching big fish off the rocks.



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