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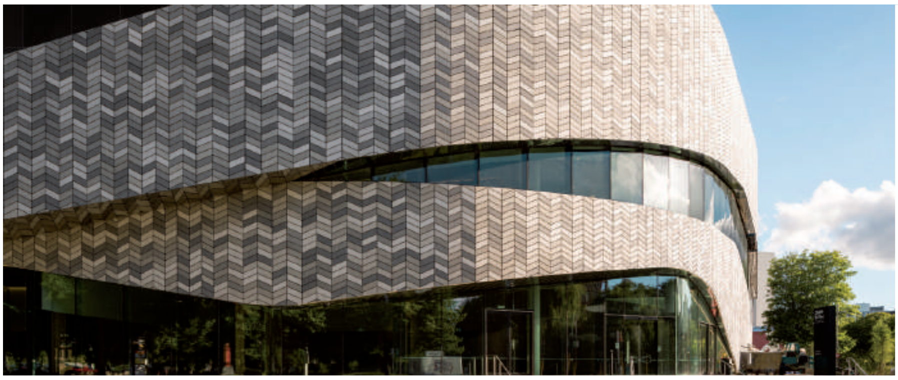

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Seminar: Design and Synthesis of Nanomaterials for Biomedical and Energy Applications

Professor Jackie Y. Ying[1]
[1]King Faisal Specialist Hospital & Research Centre, Riyadh, Saudi Arabia

Plenary Session 2, Auditorium, February 10, 2025, 08:30 - 09:30

Nanostructured materials can be designed with sophisticated features to fulfill the complex requirements of advanced material applications. Our laboratory has developed organic and inorganic nanoparticles and nanocomposites for advanced drug delivery, antimicrobial, stem cell culture, and tissue engineering applications. In addition, we have nanofabricated microfluidic systems for drug screening, in vitro toxicology, and diagnostic applications. The nanosystems allow for the rapid and automated processing of drug candidates and clinical samples in tiny volumes, greatly facilitating drug testing, genotyping assays, infectious disease detection, point-of-care monitoring, as well as cancer diagnosis and prognosis.

We have also synthesized metallic, metal oxide and semiconducting nanoclusters, nanocrystals and nanosheets of controlled dimensions and morphology. The nano-sized building blocks are used to create multifunctional systems with excellent dispersion and unique properties. Nanoporous materials of a variety of metal oxide and organic backbone have also been created with high surface areas and well-defined porosities. These nanostructured materials are successfully tailored towards energy and sustainability applications.

Molecular origin of slippery behaviour in tethered liquid layers

Professor Chiara Neto[1]
[1]The University of Sydney, Camperdwon, Australia

Keynote Session 1, Auditorium, February 10, 2025, 09:40 - 10:15

Slippery covalently-attached liquid surfaces (SCALS) with low contact angle hysteresis (CAH, <2°) and nanoscale thickness display impressive low droplet friction, which correlates with low fouling, low ice adhesion, low accumulation of scale deposits, and low friction.[1] A Goldilocks zone of lowest CAH was identified for SCALS of intermediate thickness (3.5 nm), yet, molecular-level insights are missing to reveal the underlying physical mechanism of this elusive, slippery optimum. We used advanced surface characterisation techniques to quantify the chain length and grafting density of a range of polydimethylsiloxane (PDMS) SCALS, elucidating the nanostructure responsible for their properties.[2]

More recently we used coarse-grained molecular dynamics simulations to correlated the SCALS behaviour with the quantified nanostructure. The agreement between molecular dynamics simulations and atomic force microscopy data show that nanoscale defects, as well as deformation for thicker layers, are key to explaining the existence of this `just right' regime. At low thickness values, insufficient substrate coverage gives rise to chemical patchiness; at larger thickness values, both layer waviness, previously overlooked, and layer deformation emerge, increasing contact angle hysteresis. The most pronounced slippery behaviour occurs for smooth PDMS layers that do not exhibit nanoscale waviness. The converging insights from molecular simulations, experiments, and a contact angle hysteresis theory provide design guidelines for tethered polymer layers with ultra-low contact angle hysteresis.[3]

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Ionic Materials for Next Generation Energy Technologies

Professor Doug Macfarlane[1]
[1]Monash University, Melbourne, Australia

Keynote Session 2, Dobson 1, February 10, 2025, 09:40 - 10:15

Novel materials are the key to advances in a number of energy technologies that will be critical in the transition to a Net-Zero society. This talk will discuss emerging applications of new families of ionic materials that are the basis for breakthroughs in (i) green electrochemical ammonia production, (ii) the Carnot battery and (iii) high efficiency refrigeration.

Green ammonia has become widely recognized in recent years as a potential component of the future global energy economy. Produced from renewables, N2 and water, ammonia can be viewed as an energy carrier that can be used as fuel in combustion engines, turbines and even co-firing along with other fuels. Of course, green ammonia also has an important role in displacing fossil-fuel based ammonia in the fertilizer and chemicals supply chains. In our recent work we have demonstrated a Li-mediated electrochemical process that produces NH3 at high rates with faradaic efficiencies approaching 100%. Phosphonium ionic liquids have been shown to be highly productive in this role and our studies providing some indication of the key properties that such a proton carrier must possess.

Similar ionic materials, but in their solid states, are finding application in the Carnot battery that stores energy inexpensively as heat and in high efficiency cooling technologies that promise a revolution in refrigeration.

These applications and their links to the fundamental properties of ionic materials will be summarized in this talk.

Simulating Josephson junctions one atom at a time

Karen Bayros[1], Martin Cyster[1], Jackson Smith[1], Jesse Vaitkus[1,2], Nicolas Vogt[1,2], Salvy Russo[1], Professor Jared Cole[1]

[1]RMIT University, Melbourne, Australia, [2]HQS Quantum Simulations GmbH, Karlsruhe, Germany

Keynote Session 3, Dobson 4, February 10, 2025, 09:40 - 10:15

The key component of superconducting qubits is the Josephson junction, and at the moment most of these qubits use aluminium-oxide junctions. The electronic properties of such junctions are strongly dependent on the morphology of the barrier, both at the interfaces of the superconducting leads and within the metal oxide itself. Using computational techniques we analyse both how the junctions are formed and how their electrical response depends on the junction microstructure. We perform molecular dynamics simulations of the oxidation and deposition process, in order to develop atomistic models of aluminium-oxide tunnel junctions. By simulating the fabrication process, we aim to determine what characteristics naturally emerge from the fabrication process, and how they can be controlled by modifying the fabrication conditions. To understand the electrical response of these model junctions, we capture the physics of the oxide using a three-dimensional electrostatic potential computed from molecular dynamics simulations, and then use a non-equilibrium Green's functions formalism to determine the resulting charge movement through the junction. This allows us to study the influence of oxide density, stoichiometry, defects and pin-holes on the resulting circuit response. Our results provide new insights into the influence of fabrication conditions on the electrical response of metal-oxide barriers and the performance of superconducting qubits constructed from them.

Conjugated polyelectrolytes: Their diverse applications in perovskite optoelectronic devices

Professor Han Young Woo[1]
[1]Korea University, Seoul, South Korea

Session 1A: Perovskites and optoelectronics, Auditorium, February 10, 2025, 10:45 - 12:50

Metal halide perovskites (MHPs) have captured substantial attention in the optoelectronic research community over recent decades due to their remarkable magnetic, electrical, and optical properties. These materials have been applied across a broad spectrum of technologies, including photovoltaics, light-emitting diodes (LEDs), lasers, photodetectors, field-effect transistors, and solar concentrators. To enhance the performance and stability of perovskite light-emitting diodes (PeLEDs) and perovskite solar cells (PeSCs), the integration of appropriate charge transport layers (CTLs) and/or interlayers is essential. These CTLs must have suitable energy levels to facilitate efficient charge injection and transport while effectively blocking opposite charges. Moreover, the CTL ot interlayer situated beneath and/or top of the perovskite layer is particularly critical as it greatly affects the crystal growth of the perovskite layer, the formation of interfacial defects, suppression of ion migration, and heat dissipation. In this presentation, we will introduce a novel series of conjugated polyelectrolytes (CPEs) designed to serve as ideal interfacial layers and CTLs for various PeLED and PeSC devices.

Stabilising the active perovskite phase in a hybrid glass composite

Ms Celia Chen[1], Ms Chumei Ye[1], Dr Arad Lang[1], Dr Lauren McHugh[2], Professor Thomas Bennett[1], Professor Sian Dutton[1]

[1]University Of Cambridge, Cambridge, United Kingdom, [2]University of Liverpool, Liverpool, United Kingdom

Session 1A: Perovskites and optoelectronics, Auditorium, February 10, 2025, 10:45 - 12:50

Lead halide perovskites display exceptional properties for their applications in light-emitting and energy-harvesting. However, their practical implementation is hindered by phase instability and environmental degradation. [1] The most efficient perovskites typically follow the general formula [ABX3], where the A = Cs+, methylammonium (MA, CH3NH3+) or formamdinium (FA, CH(NH2)2+), B = Pb, Sn, and X = Cl, I, Br. A critical challenge involves their intrinsic transition from the functionally active cubic α-phase to the non-functional hexagonal δ-phase under ambient conditions. [2]

A promising approach to stabilising the active phase involves encapsulating the perovskite in a hybrid inorganic-organic glass matrix. This vitreous matrix passivates the perovskite surface and imparts interfacial interactions for phase stabilisation. Additionally, the matrix serves as a protective layer, shielding the perovskite from degradation due to moisture, solvents, and light irradiation, extending its lifespan and enhancing its performance. This glass encapsulation technique has successfully stabilised CsPbI3 within the ZIF-62 glass matrix, improving photoluminescence properties for light-emitting device fabrication. [3]

Building on this success, we extend this strategy to other members of the perovskite family, particularly FAPbI3. Given the lower degradation temperature of FAPbI3, a glass matrix with a lower processing temperature is required. This work demonstrates the success of the Zn(H2PO4)2(TzH)2 (TzH = 1,2,4-triazole) hybrid glass in stabilising the active FAPbI3 phase. Resolving perovskite instability is crucial for the widespread implementation of optoelectronic devices to harness their excellent properties in bandgap tunability, emission properties, and low-cost production.

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Lead-free Organic-Inorganic Hybrid Copper Halides for Optoelectronic Applications

A/Prof Jonathan Halpert[1]
[1]The Hong Kong University of Science & Technology, Hong Kong, Hong Kong

Session 1A: Perovskites and optoelectronics, Auditorium, February 10, 2025, 10:45 - 12:50

Lead-based perovskites have advanced tremendously over the last decade, producing solar cells with PCE > 24% and LEDs with external quantum efficiency (EQE) over 20 % for both red and green. Here we report our ongoing work to improve the EQE, color and photostability of these devices. Here we will first discuss our work on perovskite red and blue emitting LEDs. However, the toxicity and instability of lead halide perovskites may still limit their applications. To address this issue, we have synthesized a novel class of copper-based micro- and nanomaterials that have high QY, up to 100%, and are long lived when packaged under nitrogen. We then show our recent work in copper-based self-trapped excitonic (STE) emitters, to produce highly luminescent, long-lived emitters with red to near-IR emission peaks. In particular, we report alkali copper(I) iodide (ACuI)-based (A = Na, K, Rb, and Cs) organic-inorganic hybrid materials with different structures and emission peaks by adjustment of the alkali atoms and organic molecules. We can also substitute bromide and chloride for pure and mixed halides, such as red emissive lead-free hybrid organic-inorganic copper halides A6(C4H8OS)12[Cu8X13] [Cu4X4(OH)(H2O)] (ACX-THTO, A = K, Rb, and Cs; X = Cl, Br; THTO = C4H8OS). These compounds possess strong photoluminescence with emission peaks in the range of 530-660 nm with a highest PLQY of nearly 100 and can be reversibly interconverted by the removal and addition of the organic components. In general, the technique for producing hybrid organic inorganic copper halides can be extended to several members of the family, with increasing stability, for the purpose of synthesizing a wide array of emissive species, covering the visible spectrum. Green, yellow, and red down-conversion light emitting devices (LEDs) can be fabricated by using these materials, and a white LED based on all-copper iodide phosphors is demonstrated with a high color rendering index (CRI) of 93 by utilizing a mixture of blue-emissive Cs3Cu2I5 and yellow-emissive Rb2Cu2I4(C4H8OS)3 powders. In addition to our work on LEDs and emissive materials, we will discuss our recent work on circular dichroism and spin selectivity in ternary non-perovskite nanocrystals.

Novel Donor-Acceptor Inverted S-T Gap Emitters for OLED Applications

Professor Przemyslaw Data[1], Mr Prasannamani Govindharaj[1], Mr Dharmendra Kumar[1], Dr Marcin Lindnder[2]
[1]Lodz University of Technology, Lodz, Poland, [2]Institute of Organic Chemistry, Polish Academy of Sciences, Warsaw, Poland

Session 1A: Perovskites and optoelectronics, Auditorium, February 10, 2025, 10:45 - 12:50

TADF OLEDs have been demonstrated with nearly 100% utilization of singlet and triplet excitons due to the efficient (reverse InterSystem Crossing) rISC processes. However, regarding material design and photophysics, the charge transfer to the induced TADF mechanism and the relaxation of the excited state in dominating the bandwidth still puzzles scientists. In most efficient TADF emitters, additional energy is needed to harvest the triplet excited state in the singlet excited state and TADF process. This is caused by the fact that the triplet energy state is always the lowest. But if we would have an inversion in such materials, there is no need for thermal up-conversion from triplet to the singlet excited state, and the RISC process should be faster than for typical TADF emitters.

Some theories on inverted S-T gap TADF OLEDs have been demonstrated in the last few years, mostly based on a rigid polycyclic aromatic framework with a para-substitution of the nitrogen atom to increase a resonant effect. We recently presented that similar behaviour is possible in CT-based donor-acceptor TADF emitters based on N-doped concave PAHs and naphthalene benzimidazoles.
Here, we would like to present entirely new donor-acceptor non-multiple resonance structures, which exhibit an inverted singlet-triplet gap. Comprehensive analysis from photophysics to OLED devices revealed very promising results and efficiencies.

Acknowledgement:
I would like to acknowledge the support received from the Polish National Science Centre project no. 2022/45/B/ST4/00800 „Ambipolar, bowl-shaped polyaromatic compounds with manifold, precisely arranged, nitrogen dopants. Unprecedented class of efficient OLED emitters”.

Electro-absorption switching of nanoplatelets

Ms Kyla Rutherford[1], Dr Harini Hapuarachchi[1], Dr Hugh Sullivan[1], Prof Jared Cole[1]
[1]Chemical and Quantum Physics, and ARC Centre of Excellence in Exciton Science, School of Science, RMIT University, Melbourne, Australia

Session 1A: Perovskites and optoelectronics, Auditorium, February 10, 2025, 10:45 - 12:50

Modern optical communication systems require compact electro-optic devices capable of swiftly altering optical properties. Nano-scale devices, such as electro-absorption (EA) modulators utilizing the quantum-confined Stark effect (QCSE) in quantum-well structures, have emerged as pivotal elements [1]. These devices serve various roles, ranging from optical interconnects for high-performance computing and data storage centres, to on-chip data links [2].

Applying an external electric field along the confinement axis, the optical absorption properties of the quantum-confined structure can be manipulated, thereby modifying the transition intensity profile [3, 4]. We apply the finite element method along with the self-consistent Schrödinger-Poisson equation to effectively model the electro-optical properties of a single exciton within nanoplatelet dimers and vertically stacked nanoplatelets while exposed to a intense electromagnetic field. Within this scheme, the electron-hole pair can undergo abrupt dissociation across the multiple quantum wells leading to enhanced electro-absorption modulation.

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Hydrogen generation with sustainable resources using a combined molecular, computational and engineering approach

Professor Keith Gordon[1], Professor James Crowley[1]
[1]University Of Otago, Dunedin, New Zealand

Session 1B: Hydrogen production and utilisation, Dobson 1, February 10, 2025, 10:45 - 12:50

Green hydrogen (hydrogen produced through renewable means) has the potential to contribute to the energy needs of the human race over the coming decades. Molecular photocatalysts offer access to green hydrogen production. These are attractive photoactive systems because they can be tuned to absorb across much the solar spectral region and from long-lived excited states that do not lead to degradation of the material. These are made up of a light harvesting part and a catalyst unit. The light harvester captures solar energy through photoexcitation to an excited state. These excited states are more effective when long-lived and the whole system has to be durable in photoreactor conditions. However there is an intrinsic flaw to this approach; it relies on rare earth metals (that are expensive, not abundant and often toxic) in the construction of the light harvester. Our hypothesis is that we can circumvent this shortcoming by using earth abundant metals in the light harvester if we utilise a different type of excited state to trap the photon energy for catalytic turn-over. We have discovered a route to long-lived excited states in which the metal plays a role but is not actually involved electronically in the final excited state – these are called intraligand charge-transfer (ILCT) states. We present ideas around how this may be accomplished.

Improvement of Photocatalytic Water Splitting activity by Facet-Selective Loading of Ultrafine Rhodium–Chromium Mixed-Oxide Cocatalyst

Yuichi Negishi[1]
[1]Tohoku University, Sendai, Japan

Session 1B: Hydrogen production and utilisation, Dobson 1, February 10, 2025, 10:45 - 12:50

The development of water-splitting photocatalysts capable of generating green hydrogen (H2) from water and sun-light is crucial for achieving carbon neutrality. Further enhancement of photocatalytic water-splitting activity is essen-tial to realizing this objective. Photocatalysts with specific exposed crystal facets can facilitate efficient charge separa-tion of electron/holes, thereby achieving high activity for water splitting. However, there have been no reports of ul-trafine (~1 nm) cocatalysts being loaded onto specific crystal facets of photocatalysts, despite cocatalysts being the actual reaction site for water splitting. This study establishes a novel method for achieving facet-selective loading of ultrafine H2-evolution cocatalysts onto the {100} facet, which is the H2-evolution facet, of a strontium titanate photo-catalyst. The resulting photocatalyst exhibits the highest apparent quantum yield achieved to date for strontium titanate. This research holds the potential to further improve various types of advanced photocatalysts and is expected to accelerate the transition to carbon neutrality.

Quinone-containing Ruthenium Complexes for Photocatalytic Hydrogen Generation

MX Winter Zakaria[1], Dr. Chris Fitchett[1]
[1]University Of Canterbury, Christchurch, New Zealand

Session 1B: Hydrogen production and utilisation, Dobson 1, February 10, 2025, 10:45 - 12:50

Artificial photosynthesis has been a desirable target of research for many years due to its potential for abundant energy production coupled with energy storage.[1] Biological systems achieve photosynthesis using highly organised architectures consisting of light-harvesting units (e.g. porphyrins), electron relays (quinones), and coupled water-splitting reaction sites (ferredoxin, Oxygen-Evolving Complex). By mimicking the functions of these units using artificial counterparts, progress on artificial photosynthesis can be achieved.

Previous research has been carried out on quinone-containing ligands complexed with ruthenium(II).[2] The MLCT absorption of these complexes has been shown to undergo consecutive quenching by transfer of an electron to the quinone moiety, essentially resulting in a photodriven reduction when coupled with a sacrificial electron donor.

Inspired by these previous examples, two novel quinone-containing ligands have been synthesised and isolated, and subsequent complexation with ruthenium(II)-containing complexes completed. These molecules are expected to have a greater reduction potential, leading to more useful energy than previous structures.

In addition to adjusting the reduction potentials of the redox-active ligand, work has been done to functionalise the ‘capping ligands’ that are auxiliary to the catalytic activity of the complex. The added functions are intended to be used as reaction sites for polymerisation via dynamic covalent bonding to form covalent organic frameworks (COFs) with the intent to transform the complex from a homogeneous catalyst to a heterogeneous one with desirable physical characteristics that are afforded by COF structures.[3]

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NiFe Catalyst Coated Membranes via Direct Membrane Deposition for High-Performance Anion Exchange Membrane Water Electrolysers

Miss Laura Titheridge[1], Professor Aaron Marshall[1], Dr Chang Wu[1]
[1]University of Canterbury, Christchurch, New Zealand

Session 1B: Hydrogen production and utilisation, Dobson 1, February 10, 2025, 10:45 - 12:50

A novel direct membrane deposition (DMD) method was developed to create a NiFe catalyst layer on an anion exchange membrane. At short deposition times, the catalyst layer was thin, sparsely distributed with finer "pom-pom"-like particles. As the deposition time increased, the layer thickened and particles transitioned through a flower-like morphology until they formed clumped structures. Whilst the initial performance of the DMD membranes was impressive, it gradually decreased over time as the catalysts were delaminating from the surface. To reduce the catalyst loss, different ionomer layer assemblies and thicknesses were investigated. As the base-layer ionomer layer thickness was increased, both cell performance and stability improved due to the roughening effect of the base-coat ionomer on the membrane, which created a catalyst layer with a higher surface area during deposition. Using too thick of an ionomer base-coat reduced the performance due to the increased thickness and diffusion limitations.

Whilst the technique can be applied both in- and ex-situ, the ex-situ method was applied in this work to allow for the optimisation of variables affecting catalyst deposition and to create pristine samples for characterisation. However, once a DMD catalyst assembly is optimised, the technique can be utilised in-situ. This could have practical implications for industrial scale-up and electrolyser manufacturing, as it simplifies the processing steps. By reducing the number of steps required for catalyst application and assembly, this approach could lead to more efficient and cost-effective production of high-performance electrolysers.

Utilisation of waste precipitated iron residues from non-ferrous hydrometallurgy in hydrogen-based ironmaking

Mr Josh McArdle[1], Professor Chris Bumby[2], Professor Aaron Marshall[1], Professor Matthew Watson[1]
[1]University of Canterbury, Christchurch, New Zealand, [2]Robinson Research Institute, Wellington, New Zealand

Session 1B: Hydrogen production and utilisation, Dobson 1, February 10, 2025, 10:45 - 12:50

Hydrogen (H_2) ironmaking can eliminate ~7% of CO_2 emissions [1]. Electrifying other fossil-intensive sectors will further reduce industrial emissions but require increased mineral extraction via hydrometallurgical processing [2]. Iron's high natural abundance necessitates removal in hydrometallurgy [3-5], often through precipitation, creating ~100 Mt/y (dry-basis Fe_2O_3-equivalent) of an unstable and toxic precipitated iron residue (PIR) by-product. This resource waste and its associated environmental damage could be mitigated by beneficiating PIR for the ironmaking industry, also addressing the decline in quality iron ore resources [6]. Utilization of PIRs for the emerging H_2-ironmaking industry is the focus of the present research. PIR was synthesized, pelletized, sintered and reduced with H_2, simulating ironmaking in a vertical shaft furnace. Using 1 wt.% of binder, pellets were formed with varied amounts of PIR and New Zealand titanomagnetite (TTM) iron sand. Physical and chemical properties of these ironmaking materials were characterized prior to laboratory-based ironmaking experiments. A first of its kind (in New Zealand) high-temperature X-ray diffraction system was set-up and used for in-situ oxidation (sintering) and H_2-reduction experiments. It was shown that increased content of PIR resulted in enhanced reduction kinetics in the pellets, however, also caused decreased sintered pellet strength and an undesirable sulphur content. A 5 wt.% PIR blend into pellets mitigated these negative effects while enhancing H_2-reduction up to 20%. Given the 2.6 Gt/y scale of iron ore processed, blending ~5 wt.% PIR into conventional ores offers a viable alternative feedstock additive for ironmaking while increasing resource recycling in mineral processing.

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Comparative Analysis of NZ Titanomagnetite and Pilbara Hematite Reduction: Influence of Preoxidation and Bed Mass on Kinetics and Morphology

Bavinesh Maisuria[1], Prof Chris Bumby[1,2], Dr Daniel Lane[4], Prof Matthew Watson[2,3]
[1]Robinson Research Institute, Wellington, New Zealand, [2]Macdiarmid Institute, [3]University of Canterbury, Christchurch, New Zealand , [4]CSIRO, Australia

Session 1B: Hydrogen production and utilisation, Dobson 1, February 10, 2025, 10:45 - 12:50

This study examines the hydrogen reduction of pre-oxidised titanomagnetite (Fe3-xTixO4) in a fluidised bed reactor, focusing on pre-oxidation effects and comparisons with Pilbara hematite. Titanomagnetite was pre-oxidised to hematite (Fe2O3) at 1000°C before reduction. We assessed the impact of preoxidation, reduction temperature, gas flow rate, and changing bed mass on reduction efficiency. Results show preoxidation enhances reduction kinetics, achieving over 90% reduction under optimal conditions.

Adjusting bed mass significantly influenced the reduction time. Compared to Pilbara hematite, titanomagnetite demonstrated distinct reduction behaviours, highlighting the benefits of pre-oxidation and operational control for sustainable iron production.

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Mechanochemical reduction of New Zealand resources to TiFe for hydrogen storage

Alexander Haack[1,2], Dr Claudio Pistidda[2], Prof Nigel Lucas[1]
[1]University of Otago, Dunedin, New Zealand, [2]Helmholtz-Zentrum Hereon, Geesthacht, Germany

Session 1B: Hydrogen production and utilisation, Dobson 1, February 10, 2025, 10:45 - 12:50

Iron-titanium-based alloys are promising materials for large-scale hydrogen storage applications.[1,2] New Zealand has large deposits of raw materials containing iron and titanium in the form of oxides; among them is ilmenite (FeTiO3). This material is a potential cheap and abundant source of hydrogen absorbing TiFe alloys. We compare the benefits and challenges of reducing ilmenite with the help of hydrogen, calcium, magnesium or a mix of these elements. A focus will be on the mechanochemical reduction in a planetary ball mill. The influence of milling parameters on the final product is discussed, as well as its washing to remove the reducing agent impurities.

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Tailored nanoporous materials for carbon capture and conversion

Dr Gurwinder Singh[1]
[1]The University of Newcastle, New Castle, Australia

Session 1C: Porous materials, Dobson 2, February 10, 2025, 10:45 - 12:50

Nanoporous materials containing pores in the nanodomains of micro (0-2 nm) and meso (2-50 nm) sizes have found extensive utilization in carbon capture and conversion which is a desired pursuit to combat the prevalent issue of CO2 emissions[1]. Micropores ideally situated near the ultramicroporous region (< 0.8 nm) are well suited for the low-pressure adsorption (post-combustion capture scenario) of CO2 molecules which possess a kinetic diameter of 0.33 nm. The mesopores play a dominant role in the adsorption of CO2 molecules at high pressure (pre-combustion scenario) via a multilayer formation and CO2 conversion by facilitating higher mass transfer. In addition to the interplay of porous structures, surface functionalization of nanoporous materials also brings in a significant advantage for CO2 adsorption, in particular at low-pressure conditions and CO2 conversion[2]. Nanoporous materials such as MOFs, zeolites, silicas, carbons and covalent organic frameworks are well-explored for such operations. Nanoporous materials such as porous carbons also offer other unique characteristics and advantages such as high surface area and large pore volume, good chemical and thermal stability and hydrophobicity which are all useful attributes for CO2 capture operations[3]. However, research challenges about facilitating an exclusive micro or meso or a hierarchical micro and meso porous structure with controlled functionalization in such materials still exist. From an application point of view, more exploratory research into the testing of CO2 adsorption under real flue stream conditions is required and for CO2 conversion, efforts should prioritize to develop materials that can facilitate the conversion via more energy-efficient pathways.

Spatially resolved gas selectivity profiles in porous adsorbents

Dr Lujia (Luke) Liu[1,2], Wenwen Liu[1,2], Zizhong Zhang[1,2], Elnaz Jangodaz[1,3], Courtney Ennis[1,4]
[1]The MacDiarmid Institute, New Zealand, [2]Victoria University of Wellington, Wellington, New Zealand, [3]Massey University, Palmerston North, New Zealand, [4]Otago University, Dunedin, New Zealand

Session 1C: Porous materials, Dobson 2, February 10, 2025, 10:45 - 12:50

Selective gas adsorption is crucial for energy-efficient gas separations, playing a pivotal role in mitigating climate change, improving energy resilience, and producing critical commodities. Understanding the structural origins of selectivity is vital for developing and refining materials with enhanced gas separation performance. However, current experimental methods for directly determining adsorption selectivity from gas mixtures are limited. Consequently, selectivity is often extrapolated indirectly from unary (single-component) adsorption isotherms. Common methods to report selectivity include: 1) Henry coefficient ratios, 2) adsorption capacity ratios at specific pressures and temperatures, and 3) ideal adsorption solution theory (IAST) selectivity. Each method has its limitations, and all report selectivity as a bulk property of a sorbent, failing to produce structure-selectivity relationships.

To gain structural insights into selectivity, researchers have developed various experimental and computational tools, including in situ single-crystal (SC-XRD) and powder X-ray diffractions (PXRD), density functional theory (DFT) calculations, and grand canonical Monte Carlo (GCMC) simulations. While these tools provide valuable structural information, none produce direct structure-selectivity relationships.

In this study, we present a novel method for producing spatially resolved selectivity profiles of gas mixtures within porous sorbents. This approach is applicable to binary, ternary, or higher-order gas/vapor mixtures and can be utilized for any type of porous sorbent, whether crystalline or amorphous. To demonstrate the method's efficacy, we report on a metal-organic framework named VUF-1 (VUF = Victoria University Framework) and use CH_4/N_2 selectivity as an illustrative example.

An upper bound visualization of design trade-offs in adsorbent materials for gas separations

Dr Matthew Cowan[1], Dr Sam J. Edens[1], Dr Gavin S. Hedley[1], Ahmed H. Elashkar[1], Dr Michael J. McGrath[1], Dr Siyu Guo[2], Dr Zijuan Du[2], Hemin Zhou[2], Dr Zuhao Shi[2], Dr Jieshuo Wan[2], Professor Thomas D. Bennett[3], Professor Ang Qiao[2], Professor Haizheng Tao[2], Professor Neng Li[2], Professor Shane Telfer[4]
[1]University Of Canterbury, Christchurch, New Zealand, [2]Wuhan University of Technology, Wuhan, China, [3]University of Cambridge, Cambridge, United Kingdom, [4]Massey University, Palmerston North, New Zealand

Session 1C: Porous materials, Dobson 2, February 10, 2025, 10:45 - 12:50

This work applies an empirical bound visualization technique, analogous to the Robeson upper bound from membrane science, to adsorbent materials proposed for gas separation and storage. [1,2]

The last 20 years have seen many publications investigating porous solids for gas adsorption and separation. The abundance of adsorbent materials (this work identifies 1608 materials for CO2/N2 separation alone) provides a challenge to obtaining a comprehensive view of the field, identifying leading design strategies, and selecting materials for process modeling.

The empirical bound visualizations described herein reveal that adsorbent materials are limited by design trade-offs between capacity, selectivity, and heat of adsorption.

We apply bound visualizations to adsorbents studied for light alkene/alkane separations and a variety of other gas pairs (CO2, H2, CH4, N2, etc.). We highlight their use in identifying candidate materials for examination within process models. Additionally, we examine the leading materials for structural design principles and guiding insights that can be applied to developing the most effective materials design strategies for metal organic frameworks and other adsorbent materials. Furthermore, we note the limitations of upper and lower bound visualizations and provide links to a database resource for researchers to produce and download bound visualization plots.

We anticipate that introducing bound visualizations to the field of metal organic framework adsorbents for gas separations will allow researchers to provide context for the importance of new materials discoveries, understand trade-offs in adsorbent design, and connect process engineers with candidate materials.

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Development of novel Hybrid Ultramicroporous Materials for Selective Gas Purification

Ms Brooke Matthews[1,2], Dr Nathan Harvey-Reid[1,2,3], Elnaz Jangodaz[2,4], Shane Telfer[2,4], Paul Kruger[1,2]
[1]University Of Canterbury, Christchurch, New Zealand, [2]The MacDiarmid Institute, Wellington, New Zealand, [3]Robinson Research Institute, Lower Hutt, Wellington, New Zealand, [4]Massey University, Palmerston North, New Zealand

Session 1C: Porous materials, Dobson 2, February 10, 2025, 10:45 - 12:50

Processes that are able to separate and purify components of chemical mixtures are of vital importance to industry. While necessary to produce vital chemical feedstock, they consume ~15 % of the world's total energy expenditure.1 Separating gases that have similar physical properties is challenging, and usually requires energy-intensive cryogenic distillation to purify.2,3 Alternative methods of purifying these challenging chemicals would significantly reduce the energy cost of producing these vital chemicals.
A sub-class of metal-organic framework (MOF) materials, hybrid ultramicroporous materials (HUMs) show promise for selecting between gases that are typically hard to separate.4,5 These materials are composed of both organic and inorganic components and have pore diameters of less than 7 Å. These narrow pore openings allow for improved selectivity, and the pore environment can be tailored through organic and inorganic component selection to allow for fine-tuning of the pore to generate affinity for the desired guest molecule.

Our research considered variations on these frameworks using a range of different transition metals, anions, and ligands to modify the pore apertures and cavity environments. The resulting frameworks were assessed for their ability to capture and separate a number of industrially relevant gases.

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Hydrogen-bonded Organic Frameworks for Selective Hydrogen Isotope Separation

Miss Edin Liu[1]
[1]Victoria University of Wellington, Wellington, New Zealand

Session 1C: Porous materials, Dobson 2, February 10, 2025, 10:45 - 12:50

Hydrogen isotope separation can be achieved through kinetic quantum sieving (KQS), which exploits confinement effects in nanoporous materials.[1] Hydrogen-bonded Organic Frameworks (HOFs), assembled through directional hydrogen bonding interactions, represent promising candidates for isotope separation due to their tunable pore, facile self-healing capability and regeneration properties.[2] In this study, we construct a series of Hexakis(isophthalic acid)benzene-based HOFs using different solvents N,N-Dimethylformamide (DMF), N,N-Dimethylacetamide (DMA), N,N-Diethylformamide (DEF), and Dimethyl sulfoxide (DMSO). These HOFs demonstrated good stability after incubation in DCM, acetone, and toluene for seven days. The structural features and thermal stability were characterized by single-crystal X-ray diffraction (SCXRD), powder X-ray diffraction (PXRD), and thermogravimetric analysis (TGA). ZEO++ revealed that DMF, DEF, DMA-derived HOF exhibited hierarchical pores (6.1-6.5 Å) in DMF-derived HOF, uniform channels (4.4 Å) in DEF-derived HOF, and a dual-pore system (4.4 Å and 6.4 Å) in DMA-derived HOF.[3] The optimal 4.4 Å pore dimension in DMA and DEF variants closely matched the quantum sieving requirements for H_2/D_2 separation(3 - 6 Å).[4]

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Highly Selective MOF Fillers in Mixed Matrix Membrane for Efficient CO2 Separation

Dr Ben Yin[1,2], Dr Shane Telfer[3], Mr Agung Pambudi[1], Dr Yiming Zhang[3]
[1]Victoria University of Wellington, Wellington, New Zealand, [2]The MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, Wellington 6140, New Zealand, Wellington, New Zealand, [3]The MacDiarmid Institute for Minerals to Materials Research, School of Fundamental Sciences, Massey University, Palmerston North, 4442, New Zealand, Palmerston North, New Zealand

Session 1C: Porous materials, Dobson 2, February 10, 2025, 10:45 - 12:50

The gas separation performance of mixed matrix membranes (MMMs) is significantly influenced by the choice of inorganic fillers. In this context, the search for new and effective fillers is vital for advancing MMM technology. Metal-organic frameworks (MOFs) have been explored extensively as superior fillers for MMMs. Despite this, there is a scarcity of high-performance MOF fillers in demand. To address this challenge, we introduce a series of novel MOF fillers with outstanding physicochemical properties, offering promising potential for MMM development.

In this presentation, we will show our efforts in creating novel mixed matrix membranes using a range of MOF fillers and their isoreticular analogues. Initial gas permeation results indicate that these new MMMs show significant promise for achieving efficient CO2 separation. We will provide updates on the latest advancements in the development of these MOF-based membranes.

Photophysics and charge-transfer states in organic semiconductors

Professor JaeHong Park[1]
[1]Ewha Womans University, Seoul, South Korea

Session 1D: Spectroscopy and applications, Dobson 3, February 10, 2025, 10:45 - 12:50

Charge-transfer states play a crucial role in photophysical processes of optoelectronic materials. Here, we present two organic semiconducting systems, where one features intramolecular charge-transfer state in covalently bound electron donor-acceptor molecule, and the other exhibits intermolecular charge-transfer state in non-covalently interacting donor-acceptor complex. At first, the excited-state relaxation dynamics of the former, a dithiophene-conjugated benzothiazole derivative (DTBz) fluorescent dye using femtosecond transient absorption spectroscopy and optical spectroscopy as well as quantum computational calculation will be discussed. Secondly, the impact of the molecular orientation engineering at the intermolecular charge transfer interface through off-site structural element will be introduced.

Advanced Ultrafast Photoluminescence Spectroscopy for Investigating Optoelectronic Materials

Dr Kai Chen[1,2,3], Mr Chao-Yang Lin[1,2,3]
[1]Robinson Research Institute, Faculty of Engineering, Victoria University of Wellington, Wellington, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, New Zealand, [3]The Dodd-Walls Centre for Photonic and Quantum Technologies, New Zealand

Session 1D: Spectroscopy and applications, Dobson 3, February 10, 2025, 10:45 - 12:50

The study of advanced optoelectronic materials demands precise characterization of their photophysical processes on ultrafast timescales. Currently, transient absorption (TA) techniques have been the standard approach for this purpose. While TA is effective, the complexity and indirect nature of its data interpretation can make it challenging to draw clear, straightforward conclusions.

For optoelectronic materials, due to their strong light-matter interactions, the emissive excited states are typically the key excitation species, and their emission properties are directly linked to application performance. Our approach leverages transient photoluminescence (PL) to investigate these materials, offering a distinct advantage in studying light-emitting applications. To this end, we have developed Transient Grating Photoluminescence Spectroscopy (TGPLS)[1, 2], which overcomes the limitations of conventional ultrafast PL methods. TGPLS delivers sub-picosecond time resolution, broadband detection, and a high signal-to-noise ratio, making it an exceptional tool for probing the emissive excited states crucial for light-emitting and laser applications.

In this presentation, we demonstrate the application of TGPLS to advanced optoelectronic materials, revealing key insights into their photoexcitation dynamics via ultrafast PL. Through several examples, we will highlight the unique capabilities of TGPLS in advancing the understanding and development of next-generation materials and devices.

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Chen K 1,2,3, Lin C 1,2,3
1 Robinson Research Institute, Faculty of Engineering, Victoria University of Wellington, Wellington, New Zealand
2 MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand
3 The Dodd-Walls Centre for Photonic and Quantum Technologies, Dunedin, New Zealand

Estimation of nanoparticle cluster size using fluorescence correlation spectroscopy towards the development of an adaptable biosensor for multi-analyte detection.

Mrs Sneha Mathew[1]
[1]Auckland University of Technology, Auckland, New Zealand

Session 1D: Spectroscopy and applications, Dobson 3, February 10, 2025, 10:45 - 12:50

Biosensors are important analytical tool in various fields including healthcare, environmental sensing, and food safety [1]. Traditional biosensors use integrated systems for identifying and reporting target molecules. However, these systems are tailored to a particular analyte and usually require significant re-engineering to detect a different analyte. To address this, we are developing a highly adaptable biosensor whose specificity can be easily modified to sense a wide range of biomolecules. Our biosensor uses quantum dots and nucleic acid aptamers, which selectively bind to specific targets. Unlike traditional sensors where all components are connected, our design separates the sensing part from the signal processing unit, making it easier to switch between different analytes. The system uses quantum dots (QDs) that are directed to form clusters in the presence of target molecules. Key to the success of this technique is the ability to distinguish QD clusters of varying size. To achieve this, we measure fluorescence correlations from single particles using a home-built spectrometer [2]. Here we present the results of our initial fluorescence correlation studies on sized-controlled QD clusters that were built using nucleic acid aptamers developed by our collaborators from the University of North Carolina at Charlotte [3,4]. These results are a proof of concept prior to the development of the complete biosensor.

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Enhanced Size Determination of Dielectric Microspheres Using Whispering Gallery Modes and Fluorescence Spectroscopy

Mrs Azizeh Alidoust Ghatar, Prof. Eric C Le Ru[1]
[1]The MacDiarmid Institute for Advanced Materials and Nanotechnology, School of Chemical and Physical Sciences, Victoria University of Wellington, Wellington, New Zealand

Session 1D: Spectroscopy and applications, Dobson 3, February 10, 2025, 10:45 - 12:50

The size determination of particles is critical in material science, environmental, and biomedical applications as it directly influences the understanding of particle behavior, stability, and interactions. This study presents an innovative approach combining Whispering Gallery Modes (WGMs) and fluorescence spectroscopy for the non-destructive and accurate determination of particle sizes in dielectric microspheres [1,2].

WGMs are very sharp optical resonances that occur when light waves travel along the circumference of a spherical microresonator, enhancing the sensitivity of size measurements. By coating polystyrene (PS) microspheres with dyes, we can detect and study the particle WGM resonances in the fluorescence spectrum of the dyes, and from them infer particle size [1-3]. To simplify the size determination, we use Mie theory to establish relationships between WGM resonance peaks and particle size, observing linear trends relative to particle radius. This technique enhances sensitivity and precision, allowing for accurate size determination of many single microspheres through fluorescence emission analysis.

Experimental results demonstrate the method's ability to detect small variations in particle size and determine full particle size distributions. This approach offers significant advantages over conventional methods [4-6], including real-time analysis, minimal sample damage, and enhanced sensitivity. The study underscores the potential of combining WGM analysis with fluorescence spectroscopy to achieve reliable particle size determination.

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High Performance Ultrafast Photoluminescence Spectroscopy Enabled by a Transient Grating Optical Gate and Multiple-plate Continuum Light Source

Professor Bo-Han Chen[1,2], Chao-Yang Lin[3,4,5], Zi-Cheng Jiang[1], Ching-Chung Huang[1], Dr. Amir Fathi[1], Dr. Kai Chen[3,4,5], Professor Shang-Da Yang[1,2,6]
[1]Institute of Photonics Technologies, National Tsing Hua University, Hsinchu City, Taiwan, [2]Department of Electrical Engineering, National Tsing Hua University, Hsinchu City, Taiwan, [3]MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand, [4]Robinson Research Institute, Faculty of Engineering, Victoria University of Wellington, Wellington, New Zealand, [5]The Dodd-Walls Centre for Photonic and Quantum Technologies, Dunedin, New Zealand, [6]College of Semiconductor Research, National Tsing Hua University, Hsinchu City, Taiwan

Session 1D: Spectroscopy and applications, Dobson 3, February 10, 2025, 10:45 - 12:50

We present a high-performance ultrafast broadband time-resolved photoluminescence (TRPL) system utilizing the transient grating photoluminescence spectroscopy (TGPLS) technique. At the heart of this system is a Kerr effect-induced transient grating (TG) optical gate, driven by high repetition rate ultrashort laser pulses at 1030 nm with micro-Joule pulse energy. This innovative setup satisfies the demands of modern spectroscopy applications by offering high sensitivity, rapid data acquisition, ultrafast time resolution, and a wide spectral window spanning from ultraviolet to near-infrared regions.

To ensure the reliability and robustness of our system, we conducted a comprehensive series of measurements after the implementation of the multiple plate compression (MPC) technique, which enabled us to achieve an instrument response function (IRF) of less than 80 femtoseconds. These tests confirmed the system's exceptional sensitivity, fast response, and broad spectral coverage, validating its capability to capture intricate photoluminescence dynamics with high precision. This advancement allows for more precise characterization of ultrafast photophysical processes in various materials, paving the way for breakthroughs in the study of exciton dynamics and energy transfer mechanisms.

In this work, we demonstrate the system's potential through detailed measurements of the laser dye DCM, highlighting its ability to capture fast and complex photoluminescence dynamics with remarkable clarity and accuracy. Our findings underscore the significant impact of this cutting-edge TRPL system on advancing research in photophysics and materials science.

Unveiling Photophysical Dynamics with a Transient Absorption System Covering the Visible to the Near-infrared

Mr Feng Wei Zong[1], Professor Bo-Han Chen[1,2], Aditi Kumar[3], Chun-Hao Li[1], Hsiao-Ching Chen[1], Professor Justin M. Hodgkiss[3,4], Kai Chen[4,5,6], Professor Shang-Da Yang[1,2,7]
[1]Institute of Photonics Technologies, National Tsing Hua University, Hsinchu City, Taiwan, [2]Department of Electrical Engineering, National Tsing Hua University, Hsinchu City, Taiwan, [3]School of Chemical and Physical Sciences, Victoria University of Wellington, Wellington, New Zealand, [4]MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand, [5]Robinson Research Institute, Faculty of Engineering, Victoria University of Wellington, Wellington, New Zealand, [6]The Dodd-Walls Centre for Photonic and Quantum Technologies, Dunedin, New Zealand, [7]College of Semiconductor Research, National Tsing Hua University, Hsinchu City, Taiwan

Session 1D: Spectroscopy and applications, Dobson 3, February 10, 2025, 10:45 - 12:50

We present a cutting-edge ultrafast transient absorption system that combines a remarkable 3-femtosecond temporal resolution with a broad detection spectral range extending from the visible to the near-infrared (600-1400 nm). This advanced system provides an unparalleled capability to explore and capture the dynamics of photophysical processes with exceptional detail. The synergy of high temporal resolution and extensive spectral coverage enables a comprehensive analysis of rapid processes and electronic transitions within complex materials.

In this study, we demonstrate the system's capabilities by investigating the photoexcitation dynamics in various morphologies of the non-fullerene acceptor Y6. Our findings reveal the intricate interplay of states, offering insights into how structural variations influence charge generation and recombination dynamics.

This research provides valuable understanding for optimizing the performance of organic photovoltaic devices. Importantly, our ultrafast transient absorption system is not limited to Y6 but is also applicable to a wide range of photovoltaic and solar materials, making it a versatile tool for advancing research in energy conversion technologies. By offering a unique combination of temporal precision and spectral bandwidth over an octave, our system sets a new standard for investigating ultrafast photophysical phenomena.

Super Resolution Scanning Electrochemical Cell Microscopy

Emily Wong[1], Dr Marc Brunet Cabré[2], Maida Costa de Oliveira[2], Prof. Paula Colavita[2], Dr Kim Mckelvey[1]
[1]Victoria University of Wellington, Wellington, New Zealand, [2]Trinity College Dublin, Dublin, Ireland

Session 1E: Innovative imaging, Dobson 4, February 10, 2025, 10:45 - 12:50

Electrochemical reactions underpin the development of a range of important zero-carbon technologies, including batteries, fuel cells, electrolysis cells and supercapacitors. Electrode surfaces, on which the electrochemical reactions occur, can contain a wide variety of active sites and domains, including defects, grain boundaries, single atoms, and local domains. These active sites and domains on the electrode surface determine the overall electrochemical response and so are important to understand if we want to develop new zero-carbon technologies. However, it is often extremely difficult to precisely measure the electrochemical activity of these active sites and domains, primarily because of their nanometer size.

Scanning electrochemical cell microscopy is the premier high-resolution electrochemical scanning probe technique that allows mapping the electrochemical response on electrode surfaces. Scanning electrochemical cell microscopy typically operates on the 100's of nanometer scale. However, even this resolution is two orders of magnitude less than that of the active sites and domains on an electrode surface.

I will discuss our recent work pushing the resolution of scanning electrochemical cell microscopy to the single nanometer scale. We have found that by carefully controlling the experimental conditions we can isolate the electrochemical response from features on an electrode surface that are below the nominal resolution of the scanning probe. We are even able to detect the electrochemical response from single atoms.

Method for quantifying slow-flow with photoacoustic imaging

Dr Jami Shepherd[1,2,3], Caitlin Smith[1,2], Dr Guillaume Renaud[4], Dr Kasper van Wijk[1,2]
[1]University Of Auckland, Auckland, New Zealand, [2]Dodd Walls Centre for Photonic and Quantum Technologies, New Zealand, [3]MacDiarmid Institute for Advanced Materials and Nanotechnology, New Zealand, [4]Delft University of Technology, Delft, The Netherlands

Session 1E: Innovative imaging, Dobson 4, February 10, 2025, 10:45 - 12:50

Blood flow quantification is an essential diagnostic tool for assessing the health of blood vessels, and has widespread relevance for applications including tissue-engineered scaffolds and tissue perfusion [1].

Ultrasound is routinely used clinically for measuring flow in large, fast-flowing blood vessels [2]. However Doppler-based methods rely on separating stationary signal from flow in the frequency domain, the former of which is dominant in ultrasound. Therefore, quantifying flow becomes virtually impossible when the flow is slow (< 1 cm/s). In contrast, photoacoustic imaging is based on optical absorption, which provides stronger contrast for blood than surrounding (stationary) tissues. As a result, photoacoustic imaging is promising for quantifying flow in slow-flow applications. We have developed a technique for quantitative flow mapping with photoacoustic imaging [3]. By analysing the flow from multiple directions in post-processing, we can compute both the magnitude and direction of the flow velocity at each pixel in an acoustic-resolution image. We will present our technique for both homogeneous and layered models (e.g. bone), including comparisons to conventional ultrasonic flow measurements. We will discuss technical and practical considerations and applications in medical imaging and beyond.

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Image analysis optimization for nanowire-based optical detection of molecules

Rubina Davtyan[1], Dr Nicklas Anttu[4], Mrs Julia Valderas-Gutiérrez[1,2], Dr Fredrik Höök[2,3], Dr Heiner Linke[1,2]
[1]Solid State Physics, Lund University, Lund, Sweden, [2]NanoLund, Lund University, Sweden, [3]Chalmers University of Technology, Gothenburg, Sweden, [4]Åbo Akademi, Turku, Finland

Session 1E: Innovative imaging, Dobson 4, February 10, 2025, 10:45 - 12:50

Semiconductor nanowires can enhance the signal of fluorescent molecules, thus significantly improving the limits of fluorescence detection in optical biosensing. In this work, we explore how the sensitivity can further be enhanced through "digital" detection of adequately spaced vertically aligned nanowires, employing single-emitter localization methods, and brightfield microscopy. Additionally, we introduce a systematic analysis pipeline aimed at harnessing this digital detection capability and evaluate its impact on detection sensitivity. Using a streptavidin-biotin assay, we demonstrate that single-emitter localization expands the dynamic range to encompass five orders of magnitude, enabling detections of concentrations ranging from 10 femtomolar to 10 nanomolar. This represents two to three orders of magnitude improvement in detection compared to methods that do not utilize single-emitter localization.

We validate our analysis framework by simulating an artificial dataset based on numerical solutions of Maxwell’s equations. Furthermore, we benchmark our results against total internal reflection fluorescence microscopy and find, in time-resolved titration experiments, that nanowires offer higher sensitivity at the lowest concentrations, attributed to a combination of higher protein capture rate and higher intensity per single protein binding event. These findings suggest promising applications of nanowires in both endpoint and time-resolved biosensing.

Characterisation of Materials for Nanomedicine by Cryo-electron microscopy – Technical Considerations

Ms Jacinta White[1], Mr Mark Greaves[1], Dr Malisja de Vries[1], Ms Jolien Bertouille[2], Dr Jiali Zhai[3], Dr Celesta Fong[1], Dr John Chiefari[1], Mr Greg Rollo-Walker[4], Dr Sarigama Rajesh[1], Dr Riley O'Shea[1]
[1]CSIRO, Clayton, Australia, [2]Vrije University, Ixelles, Belgium, [3]RMIT University, Melbourne, Australia, [4]Deakin University, Geelong, Australia

Session 1E: Innovative imaging, Dobson 4, February 10, 2025, 10:45 - 12:50

Nanomaterials are increasingly under investigation and used in therapeutics, water purification, antimicrobials, amongst others. Many biomedical applications use encapsulation to constrain and deliver therapeutic cargoes. Encapsulation mechanisms include the use of metal-organic frameworks (MOFs), liposomes and peptide or polymer gels. Characterisation during the development phase of this research is essential to determine the morphological characteristics of the cargo loading and suitability for function.

Due to the softness, high water content or delicate nature of the components, cryo-electron microscopy is a valuable tool to image the native structural state of these nanomaterials. Characterisation with minimal artefacts is critical to reduce ambiguity to understanding how a compositional change alters the structural properties and allows a more rational approach to design.

There are many technical considerations during sample preparation to be considered when working with viscous gels or multi-lipid containing preparations in cryo-TEM, and high water-content samples in cryo-SEM.

Preparation variables include:

Cryo-TEM
- Knowledge of sample composition
- Initial pre-blot sample volume
- Viscosity
- Sample mixing prior to plunging
- Rapid plunge freezing parameters
- Sample state – Firm/solid samples prepared using cryo-ultramicrotomy

Cryo-SEM
- Conductive grid choice
- Plunge sample volume
- Coolant and SEM transfer options
- Sublimation time

This presentation/paper will show how to optimise sample preparation for unambiguous, artefact-free cryo-TEM/SEM imaging of these challenging sample types, including polymer and peptide gels, polymer films and lipid rich liposome preparations.

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Metamaterial negative refractive index lens: experimental results and future pathways towards sub-wavelength resolution microwave imaging

Dr K. W. Eccleston[1], Dr I. G. Platt[1], Dr J. Nelson[1], Dr A. E.-C. Tan[1], Dr I. M. Woodhead[1], Dr Eva Anton[1]
[1]Lincoln Agritech, Christchurch, New Zealand

Session 1E: Innovative imaging, Dobson 4, February 10, 2025, 10:45 - 12:50

Negative refractive index lenses have the potential to be “perfect lenses”, offering image resolution beyond the diffraction limit of about half wavelength[1]. Negative refractive index materials require both negative permittivity and permeability, and in order to construct a perfect lens their relative values need to be both -1 at the operating frequency. Materials with this property, so called metamaterials, do not occur naturally, but can be engineered by combining discrete components of ordinary materials with positive permittivity and permeability.

While metamaterial lenses [2,3] and low loss metamaterials [4] with negative refractive index at microwave frequencies have been demonstrated previously, their application in microwave imaging systems remains largely unexplored. We recently demonstrated sub-wavelength microwave imaging at 3 GHz, using a lens made of ceramic dielectric resonators and metallic strips oriented in one direction [5,6].

This anisotropic lens design was chosen for ease of manufacturing, but causes astigmatism, restricting imaging to one dimension. This work will present an overview over experimental sub-wavelength resolution microwave imaging obtained using our anisotropic metamaterial lens, and explore pathways towards future isotropic negative refractive index metamaterials.

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Atomically precise synthesis of metal nanoparticles for catalysis

Professor Richard Tilley[1]
[1]University of New South Wales, Sydney, Australia

Keynote Session 4, Auditorium, February 10, 2025, 13:50 - 14:25

The primary challenge for high-performance nanoparticle catalysts is the atomic-level control of active sites. In this talk the evolution of state-of-the-art solvothermal synthesis of metal nanoparticle catalysis with atomic-level control will be discussed. A range of concepts will be discussed including (i) using nanoparticles with specific shapes to expose specific facets to enhance catalytic stability for oxygen evolution, (ii) how these nanoparticles can be decorated with a second metal to form islands that have strain for enhanced activity for hydrogen evolution and (iii) how island can be spread to form single atom catalysts resilient to CO poisoning for methanol oxidation. Developments in the transmission electron microscopy (TEM) atomic scale characterization of active sites will also be illustrated with the discussion of different imaging modes and how in situ TEM can be used to elucidate synthetic reaction mechanisms (Figure 1). Finally, a there will be a perspective on the future of atom-level nanoparticle catalyst design through precise control of support structure and single atom location to further elevate electrocatalytic performance.

Electrode and electrolyte design for high-performance aqueous zinc-ion batteries

Professor Zaiping Guo[1]
[1]University of Adelaide, Adelaide, Australia

Keynote Session 5, Dobson 1, February 10, 2025, 13:50 - 14:25

The rise of intermittent renewable sources, such as solar and wind, has spurred growing interest in electrical energy storage. Integrating grid-scale energy storage with renewable sources offers significant advantages in energy regulation and grid security. Zinc-based aqueous batteries (ZABs) have emerged as a promising energy storage technology for low-cost and large-scale applications due to the intrinsic safety of aqueous electrolytes and the highly desirable properties of the zinc metal anode, including its high theoretical capacity (820 mA h g−1 and 5855 mA h cm−3), low redox potential, and abundant resources.

However, the practical application of ZABs has faced challenges, including cathode degradation, uncontrollable zinc dendrite growth, and parasitic side reactions between the electrode and electrolyte, particularly under harsh conditions. In this presentation, I will discuss some of our recent advancements in enhancing the electrochemical performance of aqueous zinc ion batteries through electrode design and electrolyte optimization.

Gold ultrathin nanorods: synthesis and optical properties

Professor Tatsuya Tsukuda[1]
[1]University of Tokyo, Tokyo, Japan

Session 2A: Clusters and nanoparticles, Auditorium, February 10, 2025, 14:30 - 16:05

Gold ultrathin nanorods (Au UNRs) with diameters of 1.6–2.0 nm occupy a unique position located between plasmonic Au NRs and rod-like Au nanoclusters (NCs). We have synthesized Au UNRs with controlled aspect ratio (AR) in the range of 2.6–¬15 by one-dimensional oriented attachment of spherical Au NCs in the OA micelle [1,2]. Based on statistical analysis of aberration-corrected high-resolution transmission electron microscopy images, we propose that the Au UNRs are composed of cuboctahedral Au147 units one-dimensionally connected by twin defects [3]. Au UNRs exhibit localized surface plasmon resonance (LSPR) only in the longitudinal direction because their diameter is smaller than the Fermi wavelength of an electron (<2 nm): the longitudinal LSPR mode is red-shifted with increasing AR [2].

Recently, we found that the LSPR wavelength of Au UNRs is blue-shifted simply by mixing with Ag(I) [4].

High-resolution elemental mapping and X-ray photoemission spectroscopy of the resulting UNRs indicate that an Ag monoatomic layer is formed on the Au UNR surface by the antigalvanic reduction of Ag(I). This process allowed us to synthesize a series of Au@Ag core-shell UNRs with LSPR wavelengths in the range of 1.2–2.0 µm, which is suitable for bioapplication.

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Atomically precise clusters as the key active sites in selected materials for zero carbon systems

A/Prof Vladimir Golovko[1], Dr. Shailendra Sharma[1,2], Professor Aaron Marshall[2], Professor Gregory Metha[3]
[1]SPCS, University of Canterbury, Christchurch, New Zealand, [2]CAPE, University of Canterbury, Christchurch, New Zealand, [3]Department of Chemistry, University of Adelaide, Adelaide, Australia

Session 2A: Clusters and nanoparticles, Auditorium, February 10, 2025, 14:30 - 16:05

Synthesis of nanomaterials with precision down to one atom will be illustrated on the example of metal clusters – a class of materials with unique and strongly composition- and size-dependent properties.

Selected examples of fundamental studies of such materials as well as selected applications of such species as well-defined active sites in catalysis will be discussed in detail.

Specifically, selected studies highlighting unique electronic and structural features of clusters, including studies performed using synchrotron-based techniques will be introduced first. (1-10)

Next, catalytic hydrogen production and utilisation of hydrogen using cluster-based catalysts will be presented on several examples. (11-14)

Finally, our studies of the catalytic conversion of CO2 to more valuable and more reactive chemicals will be discussed in detail. (15, 16)

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Exploring Electronic Properties in Ligand-Interchangeable Gold Nanocluster Assemblies

Miss Emma Vincent[1,3,4], Professor Nicola Gaston[1,3], Professor Jared Cole[2,4]
[1]The University Of Auckland - Waipapa Taumata Rau, Auckland, New Zealand, [2]RMIT University, Melbourne, Australia, [3]The MacDiarmid Institute of Advanced Materials and Nanotechnology, Wellington, New Zealand, [4]ARC Centre of Excellence in Future Low-Energy Electronics Technologies, , Australia

Session 2A: Clusters and nanoparticles, Auditorium, February 10, 2025, 14:30 - 16:05

As electronic devices continue to advance, traditional silicon-based technologies are hitting their physical and practical limits, especially with challenges around miniaturisation, synthesis, reliability, and heat dissipation. This has created a pressing need to explore alternative materials that can overcome these hurdles.

Superatomic nanocluster assemblies, such as the atomically precise $Au_{32}Cl_8(P(CH_3)_3)_{12}$, offer a promising solution. Synthesised via self-assembly, these nanoclusters have tunable microstructures, with ligands surrounding the gold core that can be interchanged [1,2]. This interchangeability allows for adjustments in the microstructure, potentially altering the electronic properties. However, there remains much to learn about how the specific composition and lattice structure of these nanoclusters influence their electronic behaviour.

To address this, we've used a multiscale numerical approach that combines Density Functional Theory [3], Kinetic Monte Carlo simulations, and Graph Laplacian methods. This comprehensive approach enables a systematic exploration of how microstructural features impact the electronic behaviour of these nanoclusters. Our findings could open new avenues for exploring and utilising these materials in next-generation electronics.

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Synthesis and structural characterization of novel transition metal oxide clusters Ir3In3Sn12O14, RuIn6Sn6O16 and Ru4In2Sn20O21

Professor Tilo Söhnel[1], Dr Mohammed Abdelbassit[1], Dr Samuel Yick[1]
[1]University of Auckland, Auckland, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand

Session 2A: Clusters and nanoparticles, Auditorium, February 10, 2025, 14:30 - 16:05

A key structural feature across the stannate clusters is the formation of MSn6-octahedra filled with different transition metals, forming either isolated or one-dimensional endless chains through shared corners and edges of the [MSn6]-octahedra [1]. As the transition metal to tin ratio decreases, the coordination state of condensation increases systematically. Compounds like RuSn6[MO4]O4 (M = Si, Al, Mn, Fe, Co, Zn, Mg), where [MSn6]-octahedra do not condense, have been identified [1,2]. We have also reported new clusters of Fe(Fe3−xMnx)Si2Sn7O16 (x = 0…3) and FeMn3Ge2Sn7O16, which exhibit alternating octahedra of stannide and oxide layers as well as bridging units of (SiO4)4– and (GeO4)4–, respectively [3,4].

A group of novel cluster compounds Ir3In3Sn12O14, RuIn6Sn6O16 and Ru4In2Sn20O21 have recently been discovered, which exhibit new types of structures with proposed In+ and In+3 sites in addition to the possible oxidation states of Sn2+ and Sn1+. Out of the three cluster compounds, only RuIn6Sn6O16 contains highly ordered Sn/In sites with an alternating discrete Ru(Sn)6 octahedra encapsulated in an indium oxide layer and additional substructure formed by indium occupying a site of sevenfold coordination. Ru4In2Sn20O21 show the formation of isolated and condensed clusters RuSn6 clusters in the same compound for the first time. So far, only either isolated or condensed clusters could be found in a compound. Ru4In2Sn20O21 could be seen as a combination of Ru3Sn15O14 and a (hypothetical) RuSn6[SnO4]O4. Ir3In3Sn12O14 crystallizes in the Ru3Sn15O14 structure type.

The presentation will summarize the preparation and characterisation of these interesting novel materials.

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Tuning the Electronic Properties of Doped Graphullerite – a Covalently Bonded form of C60

Mr Alex Barnes[1], Dr. Stephanie Lambie[1,2], Prof. Nicola Gaston[1]
[1]MacDiarmid Institute for Advanced Materials and Nanotechnology, Department of Physics, University of Auckland, Auckland, New Zealand, [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

Session 2A: Clusters and nanoparticles, Auditorium, February 10, 2025, 14:30 - 16:05

Carbon has an abundance of allotropes, with the most well known being graphite and diamond. Two novel allotropes that have been recently synthesised are Graphullerite and Graphullerene[1]. Within Graphullerene, C_{60} buckminsterfullerenes are covalently bonded in a hexagonal pattern forming a two-dimensional sheet. These sheets then stack due to van der Waals (vdW) interactions forming Graphullerite.

Graphullerite can be doped with ions to alter its properties, and Mg_4C_{60} has been experimentally produced as a precursor during Graphullerite synthesis[1].

Our work is a computational investigation of Mg doped Graphullerite, to understand how the doping affects both the geometric and electronic properties. The experimental Mg_4C_{60} structure was used to benchmark the DFT study (within VASP) and select an appropriate Exchange Correlation functional and vdW correction. Different permutations of Mg_3C_{60}, Mg_2C_{60} and MgC_{60} were produced by removing Mg from Mg_4C_{60}. In total including Graphullerite, 50 structures were modelled allowing us to be confident that we found the lowest energy structure for each doping amount as well as having enough structures to understand the system holistically. This holistic approach was important to understand the interplay between geometry and electronics. Density of states was calculated for each structure revealing a complex zoo of electronic materials, from Semiconductors with a bandgap of 0eV to 0.20eV (under-estimated due to DFT), materials with low occupancy at the fermi level (referred to as Semi-metals), to Metallic materials.

Our geometric analysis demonstrated that doping Graphullerite can lead to drastic changes in the vdW stacking direction and the ion-ion interactions between dopants.

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Modified carbon black and NMC for improved lithium-ion battery performance

Mr Donghyuck Park[1], Professor Amanda Ellis[1]
[1]The Department of Chemical Engineering, The University Of Melbourne, Melbourne, Australia

Session 2B: Batteries and capacitors, Dobson 1, February 10, 2025, 14:30 - 16:05

Lithium-ion batteries (LiBs) are the predominant commercial form of rechargeable batteries, and their performance relies on the effectiveness of the cathode which can influence its capacity, lifespan, and charging rate. This talk will focus on improving the performance of both the conductive additive, carbon black (CB), and the active material, nickel manganese cobalt oxide (NMC), in the cathodes of LiBs. By modifying CB with carbonyl moieties, the energy barrier for lithium-ion movement at the electrode-electrolyte interface was shown to be reduced, resulting in lower overpotentials and faster charge/discharge reactions. In addition, NMC particles were modified with nanolayers of an iron-based metal phenolic network (MPN) with electrochemical impedance spectroscopy (EIS) showing improved lithium-ion accessibility to the NMC. This accessibility improves electrochemical kinetic processes within the cathode electrode, achieved through (1) improved passage of the ions in the electrolyte that penetrates the porous electrode structure (ionic transport), (2) improved passage of the ions through the cathode-electrolyte interphase, (3) improved charge-transfer reactions, and (4) improved passage of the ions in the NMC (solid-state diffusion). As a result, the cathode electrode showed reduced interfacial resistance and a more efficient NMC structural phase transition, with uniform (de)intercalation of lithium-ions on the surface. Overall, the chemical modifications of the CB and NMC lower the battery overpotential and thus the battery energy requirements, resulting in more efficient batteries.

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Enabling soft polymers as solid polymer electrolytes for Lithium metal batteries by reinforcing mechanical properties

Professor Mukundan Thelakkat[1]
[1]University Of Bayreuth, Bayreuth, Germany

Session 2B: Batteries and capacitors, Dobson 1, February 10, 2025, 14:30 - 16:05

A key theme running through the research activities of Thelakkat group concerns with diverse research topics on energy conversion and storage. The presentation gives an account of materials design and materials requirement for some of these specific applications with an emphasis on tailored polymer synthesis, characterization and testing in prototype devices. Each application has a different catalogue of material profile; some of which can be taken into account in the molecule design itself. A final structure-property relation was obtained by understanding the performance of the synthesized polymers in relevant applications. The field of conjugated and conducting polymers cover the topics of OLEDs, OFETs, Solar cells, and Thermoelectrics, whereas mixed ion-electron conductors find applications in bioelectronics. For battery applications, ion-conductors were designed and their suitability in all-solid-state batteries were elucidated. In this talk, different strategies for the design, synthesis and application of solid polymer electrolytes for lithium metal batteries will be presented. This include, bottlebrush polymers, their nanocomposites, semiinterpenetrating networks and well as block copolymers which combine both high ionic conductivity as well as sufficient mechanical properties. A general comparison of different mechanical reinforcement strategies of soft polymer materials to enable them for long term cycling in lithium metal batteries will also be presented.

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Converting Waste Woody Materials into Heteroatom-doped Electrode Materials for Electrochemical Energy Storage

Muge Ding[1], Qicheng Zhang[1], Dr Shanghai Wei[1], Professor Wei Gao[1]
[1]The University of Auckland, Auckland, New Zealand

Session 2B: Batteries and capacitors, Dobson 1, February 10, 2025, 14:30 - 16:05

Slash is a waste product from commercial forestry. When cyclone Gabrielle directly passed Hawke's Bay regions in 2022, the flooding slash caused devastating damage. Recently, we have conducted numerous experiments aimed at converting New Zealand forestry slash into high-performance electrode materials. In this presentation, we will report the research progress in converting commercial forestry waste into heteroatom-doped carbon materials. These doped materials have demonstrated excellent electrochemical energy storage properties in both supercapacitors and batteries. For example, sulfur-doped carbon materials exhibit a high capacitance of 148 $F\cdot g^{-1}$ at a current density of 0.5 $A\cdot g^{-1}$. The coin-cell supercapacitor device also shows impressive rate performance, with a maximum capacitance of 384 $F\cdot g^{-1}$ and retention of 360 $F\cdot g^{-1}$ after 10,000 cycles.

Biocompatible supercapacitor engineered from marine collagen impregnated with polypyrrole and tungsten disulfide

Dr Roshan Khadka[1]
[1]Plant & Food Research, Auckland, New Zealand

Session 2B: Batteries and capacitors, Dobson 1, February 10, 2025, 14:30 - 16:05

There is an urgent demand for highly stable energy storage systems that are biocompatible, environmentally friendly, and made from affordable, sustainable materials. Research on biologically sourced materials as green energy storage devices such as supercapacitor (SC) technologies are emerging, but they are often expensive, complicated to manufacture and fail to meet the required performance levels. We present a simple and innovative method to fabricate a human skin comfortable SC electrode using collagen extracted from hoki (Macruronus novaezelandiae) fish skin. Polypyrrole and tungsten disulfide nanoparticles were incorporated into the collagen matrix via early wetness impregnation to provide the required electrical properties. Electrochemical investigations revealed that the areal capacitance of the composite material was 348 mF cm− 2 and cyclic testing showed that the capacitance retention is 98 % after 50,000 cycles. The collagen-based composite demonstrated excellent biocompatibility to HEK293 cells grown over a 1-week period. This novel technique for producing biodegradable and biocompatible SC electrodes from renewable source paves opportunities to utilize other sources of biomaterials for smart electronic applications

Active site engineered nanozymes for advanced biosensing and beyond

Professor Moon Il Kim[1]
[1]Gachon University, Seongnam, South Korea

Session 2C: Biosensors, Dobson 2, February 10, 2025, 14:30 - 16:05

Recently, nanozymes have been intensively studied due to their superior enzyme-like qualities. In this presentation, I will discuss the current progresses how to develop active site engineered nanozymes and their representative applications in biosensing technology. First, I will describe carbon-based nanozymes, N & B-codoped graphene (NB-rGO), Fe-N4 and Cu-N4S single site embedded graphene (Fe-N-rGO and Cu-NS-rGO), which showed high peroxidase-like activity without oxidase-like activity. All the active site-engineered rGO nanozymes had dramatically high catalytic efficiencies, showing the synergistic effects of doped elements at single atom sites, increasing electron transfer during the catalytic reaction. The rGO-based nanozymes were successfully used in biosensing systems for detecting important physiological biomarkers with high selectivity and sensitivity. Then, I will introduce the development of Co-doped mesoporous cerium oxide (Co-m-ceria), which operated optimally at a near-neutral pH and exhibited a peroxidase-like catalytic efficiency over 600-fold higher than that of pristine m-ceria. Five different oxidative enzymes were immobilized in the pores of Co-m-ceria at high loadings, followed by incorporation of the enzyme-containing Co-m-ceria in paper microfluidic devices for the convenient and simultaneous detection of multiple biomarkers. Finally, I will describe laccase-like DNA-copper hybrid nanoflowers and their successful application for colorimetric detection of phenolic compounds in paper microfluidic devices. These achievements should accelerate and widen the utility of nanozymes as next-generation alternatives to natural enzymes for biosensing and beyond.

Continuous Biomolecular Monitoring Using Molecularly Responsive Hydrogel Plasmonic Biosensor

Dr Soohyun Park[1], Dr Khulan Sergelen[2]
[1]BioMed X Institute, Heidelberg, Germany, [2]BioMed X Institute, Heidelberg, Germany

Session 2C: Biosensors, Dobson 2, February 10, 2025, 14:30 - 16:05

Continuous biomolecular monitoring for long-term implantable devices demands robust, biocompatible sensors capable of consistent and reversible detection. This study presents an advanced biosensing platform utilizing aptamer crosslinked hydrogels (aptagels) engineered using multi-arm macromers.

Comprehensive analysis employing multi-parametric surface plasmon resonance (MP-SPR) and quartz crystal microbalance with dissipation monitoring (QCM-D) demonstrates that aptagels crosslinked with dual-end attached aptamers exhibit superior performance, attributed to the reversible formation of analyte-induced ternary complexes, resulting in pronounced conformational changes with localized network contraction. Systematic screening of various aptagel formulations and engineered aptamers reveals that optimizing spatial distribution of crosslinks and aptamer sequences is crucial for ensuring conformational changes and dynamic actuation of the gel network. Notably, dose-response analysis demonstrates a significantly lower limit of detection for the aptagel compared to monolayer systems, with a broad linear sensing range. Furthermore, long-term stability tests in diluted plasma confirm that the aptagel maintains specificity and stability over two weeks without signal deterioration. This aptagel-based biosensing platform offers a promising avenue for advancing in vivo biomolecular monitoring devices across diverse healthcare and research applications.

An Electrochemical Aptasensor for Detection of Cancer Biomarkers and Extracellular Vesicles

Dr Zarinah Amin[1], Professor Volker Nock[2], Dr Paula Brooksby[2], Dr Renee Goreham[1]
[1]University Of Newcastle, Newcastle, Australia, [2]University of Canterbury, Christchurch, New Zealand

Session 2C: Biosensors, Dobson 2, February 10, 2025, 14:30 - 16:05

Symptoms of lung cancer seldom manifest until the disease is already in its advanced stage. This makes it extremely hard to detect and survival chances are weak. Early diagnosis is desired to improve a patient's survival and quality of life. Nature's own nanoparticles, known as extracellular vesicles (EV), offer a promising alternative as they have proven potential for novel biomedical applications. They are nano-sized particles released by all cells and are found in various bodily fluids. As they inherit and transport "cargo" molecules such as transmembrane proteins from their cells of origin, they are useful as biomarkers.

In this project, we devised an electrochemical biosensor platform to capture EVs by using aptamers immobilised on gold surfaces. This modification rendered the surfaces useful as sensing electrodes in electrochemical impedance spectroscopy (EIS) measurements. Using optimised platforms, capture of EV generated successive calibration plots with low detection limits of < 10 particles per mL. Cancer-derived EVs were detected in vitro using a cancer-specific aptamer. Complementary data from surface plasmon resonance and circular dichroism spectroscopy measurements further confirmed binding, indicating a target-induced mechanism.

To explore further, a portable, miniaturised prototype was fabricated by transfer of the platform to a planar gold electrode pattern using photolithography. Lung cancer-derived EVs were detected in a shorter time using a tiny sample volume. The aptasensor offers an alternative route for non-invasive lung cancer screening. In contrast to current methods such as biopsy and bronchoscopy, further development could see our platform integrated into a disease breathalyser.

Implantable bioelectronics for in vivo and long-term measurement of potassium ions in pine xylem sap

Dr Yi Chen[1], Dr Dalila Pasquini[1], Dr Mathias Sorieul[1], Prof Sanggil Han[2], Prof George Malliaras[3]
[1]Scion, Rotorua, New Zealand, [2]Department of Nano-Bioengineering, Incheon National University, Incheon, Republic of Korea, [3]Electrical Engineering Division, Department of Engineering, University of Cambridge, Cambridge, UK

Session 2C: Biosensors, Dobson 2, February 10, 2025, 14:30 - 16:05

Plant growth is the sum of the response to environmental stimuli and resource availability. The challenge in monitoring the health status of individual trees lies in the ability to continuously monitor internal physiological parameters in real-time over a long period. The field of bioelectronics, such as organic electrochemical transistor (OECT) sensor has witnessed the rapid development of miniaturised in vivo implantable sensors minimising wound damage [1-2]. By leveraging the high sensitivity of OECT sensor [3] and the specificity of ion-selective membranes [4], our team successfully fabricated a potassium ion OECT sensor with a high current sensitivity (up to 270 µA/decade) and a low limit of detection (1×10-5 M). Our miniaturised sensor can easily be implanted in planta to monitor the potassium cation concentration in softwood (radiata pine) xylem. We demonstrated that this sensor provides real-time (every 10 s) measurement of in vivo xylem's sap potassium ions concentration over hundred days.

We anticipate that the outcome of this work will help to address fundamental plant physiology questions related to the cycles of this cation between foliage and root (Potassium battery concept). We foresee the impact of this research will be to enable new tools to monitor plant health for the digitalisation of forest nurseries, precision agro-forestry and horticulture (e.g. kiwi fruit and grape vine).

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Tailoring antiferromagnetic spin textures using magnetoelectric BiFeO3

Dr Vincent Garcia[1]
[1]Laboratoire Albert Fert, Palaiseau, France

Session 2D: Ferro-magnetic, ferro-electric and magnetic materials, Dobson 3, February 10, 2025, 14:30 - 16:05

Antiferromagnetic materials are emerging as a new paradigm for spintronics as they offer key advantages over ferromagnets: insensitivity to external magnetic fields, THz spin dynamics, and higher density packing.

For skyrmionics, where information is encoded in topological spin structures, antiferromagnetic skyrmions would also benefit from the absence of gyrotropic forces, giving rise to ideal fast and straight motions along the driving forces. While complex topological objects were recently discovered in intrinsic antiferromagnets, mastering their nucleation, stabilization, and manipulation with energy-efficient means remain to be demonstrated. As antiferromagnets are insensitive to external magnetic fields, one must find alternative ways to control them. Using magnetoelectric antiferromagnetic multiferroics, a low energy electric-field control of antiferromagnetism could be achieved. We take advantage of the room-temperature magnetoelectric coupling in epitaxial thin films of multiferroic $BiFeO_3$ to deterministically control antiferromagnetic spin textures via the ferroelectric domains. We design model systems containing a single ferroelectric domain coupled to a single antiferromagnetic domain, opening further opportunities for investigations of the interplay between non-collinear antiferromagnetic orders and magnon excitations.

In standard striped ferroelectric domains in $BiFeO_3$ thin films, we use epitaxial strain to finely tune the as-grown spin textures going from cycloidal to collinear states. Finally, in submicron devices based on $BiFeO_3$, we stabilize topological centre polar states using a radial electric field. We show that such polar textures can contain flux closure of antiferromagnetic spin cycloids or quadrant of canted antiferromagnetic domains, depending on the epitaxial strain. These results open the way for electrically-reconfigurable antiferromagnetic topological objects.

Grain Boundary Complexion Transitions in Ferroelectrics

Professor Catherine Bishop[1,2], Professor R. Edwin García[3], Dr K.S.N. Vikrant[4]
[1]University of Canterbury, Christchurch, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, Christchurch, New Zealand, [3]Purdue University, West Lafayette, USA, [4]IIT-Delhi, Delhi, India

Session 2D: Ferro-magnetic, ferro-electric and magnetic materials, Dobson 3, February 10, 2025, 14:30 - 16:05

Grain boundaries are distinct from domain walls in ferroelectric materials because they are characterised by both crystallographic misorientation and polarisation misorientation. [1] The aim of this work is to elucidate the equilibrium grain boundary states as a function of the two misorientations and temperature in ferroelectric bi-crystals.

Here a critical point wetting analysis of tilt grain boundaries in tetragonal ferroelectrics is presented and transitions in grain boundary core order and polarisation are identified. [2] While previous authors [3–5] have been inspired by Cahn's original critical point wetting analysis, [6] this is the first application to vector fields, where the bulk and grain boundary core contributions to energetics are both a function of the misorientations. Twist grain boundaries in ferroelectrics, where macroscopic polarisation charge is zero, are also analysed.

Further, numerical predictions of grain boundary complexion for tilt grain boundaries suggest that in-phase (head-to-tail-like) polarisation misorientations have ferroelectric grain boundary cores with a Schottky potential that could limit switching. [7] In contrast, out-of-phase (head-to-head-like) polarisation misorientations have weakly-ferroelectric grain boundary cores and no built-in electric field.

The implications of this approach for polycrystalline ferroelectrics are discussed. [8] In contrast to previous studies, [9–12] where all grain boundaries are given the same 'width' and properties, here the grain boundary state is solved self-consistently and is determined for each grain boundary independently.

Realistic grain size distributions, textures and grain boundary character distributions can be embedded in phase-field simulations to explore temperature and field effects in these interesting materials.

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Fast spin precession in ferrimagnetic Mn4N thin films with perpendicular magnetic anisotropy

Dr Yao Zhang[1]
[1]Victoria University of Wellington, Wellington, New Zealand

Session 2D: Ferro-magnetic, ferro-electric and magnetic materials, Dobson 3, February 10, 2025, 14:30 - 16:05

Ferrimagnets composed of two antiferromagnetically-coupled magnetic sublattices have attracted much attention recently due to the easily controlled and detected net magnetization and a fast magnetic dynamic behavior [1]. In particular, ferrimagnetic thin films with perpendicular magnetic anisotropy (PMA) show great potential for high-density spintronics devices [2]. Currently, most work focuses on rare earth-transition metal ferrimagnetic alloys such as GdFeCo and TbCo. However, the magnetization of these materials is sensitive to temperature and composition [3]. Antiperovskite Mn4N is a rare-earth-free ferrimagnet with PMA, high thermal stability (TC = 740 K), high spin polarization and low saturation magnetization, all highly attractive qualities for practical spintronics devices [4].

Crystalline thin films of Mn4N have previously been deposited on MgO substrates, however there is a large lattice mismatch of -6% [5]. Here, we introduced a Pd buffer layer to improve the lattice matching and perpendicular magnetic anisotropy of the Mn4N films. We prepared stacks of MgO(substrate)/Pd(t = 0, 2 and 8 nm)/Mn4N(80 nm)/Ta(3 nm) by reactive magnetron sputtering. The Pd buffer layer results in a higher crystalline quality Mn4N film with lower tetragonal distortion. The magnetisation is reduced with increasing Pd buffer layer thickness, however the coercive field is increased from ~ 400 mT to ~ 800 mT, resulting from an enhancement of PMA. Time-resolved magneto-optical Kerr effect (TR-MOKE) measurements show a fast precessional frequency of ~ 100 GHz and a high damping ~ 0.2, potentially useful for fast-switching magnetic structures.

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Electronic Structure and Electrical/Magnetic Behavior of 2D-Stanene (Stanene-Oxide) Thin Film

Professor Sekhar Ray[1]
[1]Siksha O Anusandhan Deemed to be University, Bhubaneswar, India, [2]University of South Africa, Johannesburg, South Africa

Session 2D: Ferro-magnetic, ferro-electric and magnetic materials, Dobson 3, February 10, 2025, 14:30 - 16:05

In-situ Ar+-ion etching process was used to extract the stanene/Stanene-oxide from SnOx thin film. On the process of etching (τetch = 0-4000 sec) the thickness of SnOx ≈200 nm is reduced to ≈2.5 nm and formed 2D-Stanene. X-ray photoelectron (XPS) and ultraviolet photoemission spectroscopy (UPS) were measured in-situ and confirmed the formation of different crystal structures of defect-induced 2D-stanene and/or 2D-stanene oxide ultra-thin films. The ex-situ Raman spectra measurements and X-ray absorption near edge structure (XANES) spectroscopy, further confirmed the formation of 2D-stanene/stanene-oxide. We have studied the electronic structure and electrical/magnetic behaviours of extracted 2D-stanene/stanene-oxide nanostructured materials. This in-situ Ar+-ion etching process provides a new direction to fabricate device-based 2D-stanene/stanene-oxide materials for future different electronic devices.

Terahertz spin-based sensors design

Dr Dominik Legut[1,2], Dr. Ievgenia Korniienko[1], Dr. Pablo Nieves[3], Oksana Chubykalo-Fesenko[4]
[1]Vsb - Technical University Of Ostrava, Ostrava, Czech Republic, [2]Charles University, Prague, Czech Republic, [3]Universidad de Oviedo, Oviedo, Spain, [4]ICMM–CSIC, Madrid, Spain

Session 2D: Ferro-magnetic, ferro-electric and magnetic materials, Dobson 3, February 10, 2025, 14:30 - 16:05

Based on the idea of creating sensors sensitive to the magnetic component of terahertz electromagnetic radiation, we derived a convenient analytical description of an ultrashort terahertz pulse and performed an analysis of the influence of this pulse on the Zeeman torque dynamics that are extremely important tasks due to the potential applications of terahertz radiation. The theoretical expressions proposed in this talk clarify the physics of magnetic dynamics under the action of the magnetic field of a terahertz pulse and show the role of individual parameters of the material and the pulse field in this process. On the basis of the formulas obtained and the available experimental data for fcc-Co film, we analyze the possibilities of recovering information about the magnetic field of the pulse from the observation of magnetization dynamics, as well as the effect of fluence, Gilbert damping, and magnetic anisotropy on the magnetization dynamics induced by ultrashort terahertz radiation[1]. We have advanced our theoretical understanding of Zeeman torque response to THz magnetic fieldi, made the analytic models general in order to control the magnetism over other ferromagnetic materials and determine possible candidates for creating the spin-based THz sensors, and analyze the difficulties and limitations that appear when using different types of ferromagnets, including situations out of equilibrium[2].

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Frictionless nanohighways in Bismuthene/Graphite

Dr Maxime Le Ster[1], Dr Maciej Rogala[1], Dr Iaroslav Lutsyk[1], Dr Krzysztof Podlaski[1], Dr Tevfik O. Mendeş[2], Dr Andrea Locatelli[2], Prof Simon A. Brown[3], Dr Paweł Kowalczyk[1]
[1]University Of Lodz, Łódź, Poland, [2]Elettra-Sincrotrone, Trieste, Italy, [3]The MacDiarmid Institute, University of Canterbury, Christchurch, New Zealand

Session 2E: Materials for low energy systems and computing, Dobson 4, February 10, 2025, 14:30 - 16:05

Van der Waals heterostructures offer tuneable platforms to realize frictionless contacts in a special regime of motion called structural superlubricity [1]. So far, most experimental work has focused on atomically-thin layers with hexagonal or triangular lattice symmetries, leading to isotropic frictionless properties, yet away from the energy minimum. In this talk, I will present our low-energy electron diffraction (LEED) and microscopy (LEEM) results of the α-bismuthene (Bi) on graphite system, which reveal a new regime of anisotropic frictionless contact at the energy minimum, enabled by the broken rotational symmetry of the coupled crystalline layers. The Bi islands spontaneously move back-and-forth along one-dimensional channels over distances of up to 600 nm at room temperature, even for islands comprised of up to ~10^6 atoms. Our results are supported by registry index simulations, realizing directional superlubricity [2] for the first time in a two-dimensional system. Additionally, the analysis of the Bi islands dynamics (flight and stopping times) highlight a heavy-tailed Lévy-flight-like process [3], notoriously rare in condensed-matter physics.

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Disordered Materials for Low Energy Electronics

Dr Julie Karel[1]
[1]Monash University, Melbourne, Australia

Session 2E: Materials for low energy systems and computing, Dobson 4, February 10, 2025, 14:30 - 16:05

Much of our understanding of the electronic properties of materials relies on the existence of a periodic crystal structure. A periodic lattice and in particular reciprocal space (k space) allow for a straightforward way to think about and characterise materials as well as predict their properties. In the past decade, there have been intense research efforts in topological materials, such as topological insulators, where the physical properties of the material are governed by topology in the electronic band structure. These materials exhibit exotic effects such as dissipationless transport (e.g. electrical current conduction with no resistance), making them compelling in low energy electronics.

Given their promising properties, significant work has gone into discovering and developing new topological materials, although efforts have focused almost exclusively on crystalline materials. Despite mounting theoretical predictions suggesting amorphous materials can host topological properties, this class of materials has been largely overlooked. What is more, amorphous materials are generally low cost, defect tolerant and require less energy to synthesise than their crystalline counterparts. This talk will present examples from my own work, where I will show that topological effects are important in governing the properties of disordered materials. I will highlight the potential of these materials in emerging low energy electronic and data storage devices.

Thin Film Growth of Co2MnGexGa1-x Heusler Alloys and Study of Their Structural, Electrical, and Magnetic Properties

Mr Brijeshkumar Patel[1,2], Dr Yao Zhang[1], Dr Simon Granville[1,2]
[1]Robinson Research Institute, Victoria University Of Wellington, Lower Hutt, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, New Zealand

Session 2E: Materials for low energy systems and computing, Dobson 4, February 10, 2025, 14:30 - 16:05

Ferromagnetic Heusler alloys have various applications like magnetic memory devices and spintronic applications and, their compositional tuning also provides a way to optimize particular properties for technological needs [1]. For example, compositional tuning of Co2MnGe (shows high spin polarisation [2]) and Co2MnGa (shows high anomalous Hall effect [2]) should help to achieve both properties simultaneously with high Curie temperature for Co2MnGexGa1-x. There has been no research work reported regarding Co2MnGexGa1-x thin film compared to Co2MnGe and Co2MnGa thin films. Therefore, the exploitation of topological electronic properties of Co2MnGexGa1-x thin films makes it promising for practical spintronic devices.

Here, I will present work on the successful modification of composition between Co2MnGa and Co2MnGe in thin films made via the magnetron sputtering technique on MgO (001) substrate with co-sputtering of targets. Moreover, XRD confirmed all films are in the ideal Heusler L21 structure with lattice parameters varying from 5.763 Å for Co2MnGe to 5.760 Å for Co2MnGa. Magnetic and electrical properties vary smoothly as Ge% increases from 0 to 100; saturation magnetization (at 10 K) increases from 727 emu/cc to 875 emu/cc, resistivity (at 300 K) decreases from 170 μΩcm to 22 μΩcm and anomalous Hall resistivity (at 300 K) decreases from 6.63 μΩcm to 0.03 μΩcm.

The overall work suggests the simultaneous optimization of properties such as spin polarisation and anomalous Hall effect are feasible for Co2MnGexGa1-x and other Heusler alloy systems.

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Zero Angular Momentum compensation in Rare Earth Nitrides

Ms Elma Joshy[1,2], Dr Jackson Miller[1], Dr Simon Granville[1,2]
[1]Robinson Research Institute, Victoria University of Wellington, Lower Hutt, New Zealand, [2]The MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand

Session 2E: Materials for low energy systems and computing, Dobson 4, February 10, 2025, 14:30 - 16:05

Rare earth nitrides (RENs), exhibit a set of unique properties where their distinctive combinations enable them to function as ferromagnetic semiconductors, particularly suitable for spintronics applications as cryogenic memory elements [1]. The solid solution GdxSm1-xN is promising because GdN is spin dominant with a saturation magnetisation of 7 µB/ion and SmN is orbital dominant with a very small magnetic moment of 0.035 µB/ion. The ferromagnetic exchange interaction aligns the spins of Gd3+ and Sm3+ ions, resulting in the opposition of total angular momentum for each ion in the solid solution [2]. This leads to magnetisation compensation and angular momentum compensation in the solid solution.

A series of GdxSm1-xN thin films has been grown in an ultra-high vacuum environment, and their structural properties have been studied using X-ray diffraction (XRD). The composition of Gd and Sm in the solid solution was determined by using X-Ray Fluorescence (XRF) and magnetometry has been used to study the magnetic properties of the films. The results show that magnetic saturation increases, and the coercive field decreases as the Gd content in the GdxSm1-xN solution increases. The magneto-transport measurements of the solid solutions indicate changes with the introduction of Gd ions in SmN due to the large spin magnetization of GdN which shows a negative sign for anomalous Hall effect (AHE) resistivity[3].

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Self-compensated memory structures with superconducting readout

Dr Jackson Miller[1], Dr Will Holmes-Hewett[1], Dr Simon Granville[1], A/Prof Ben Ruck[2]
[1]Paihau-Robinson Research Institute, Lower Hutt, New Zealand, [2]School of Chemical and Physical Sciences, Wellington, New Zealand

Session 2E: Materials for low energy systems and computing, Dobson 4, February 10, 2025, 14:30 - 16:05

Future computing, both classical and quantum, will be performed using superconducting electronics at low temperature. The most recent single flux quantum based logic systems have demonstrated clock-speeds of 10s of GHz, and switching energies as low as eJ, while companies such as Google and IBM are continuing to increase their logical qubit count, with the aggressive scaling so far meeting projections. However, for the promised advances of these technologies to be realised a dense, cryogenic memory must be developed.

Here, we present our work forming such a prototype superconducting memory device comprising ferromagnetic rare-earth nitrides and conventional Josephson junctions. The combination and competition of spin and unquenched orbital angular momentum on the trivalent lanthanide ions allow the tuning of various magnetic properties, to a much greater degree than in transition-metal based ferromagnets. Using combinations of (GdSm)N we demonstrate independent control of the net-magnetisation and coercive field. We show the incorporation of these layers into tri-layer structures and the formation micron-scale switchable magnetic dots. The fringe field of these dots is determined by the relative orientation of the ferromagnetic layers. The dots can affect the superconducting state of a nearby Josephson junction, which is used for electrical readout of the memory state, forming a micron-scale superconducting memory device.

Strengthening and toughening mechanisms of lightweight high-temperature high Nb-TiAl alloys using nanoscale-silicides

Dr Jun Cao[1], Professor Yongfeng Liang[1], Professor Junpin Lin[1]
[1]University of Science and Technology Beijing, Beijing, P.R. of China

Session 3A: Alloys, ceramics and oxides, Auditorium, February 10, 2025, 16:35 - 17:55

TiAl alloys, having low density, high strength, high stiffness and good oxidation resistance, are used in the GE90 series of large-containment-ratio turbofan aircraft engines built by General Electric (GE) for the Boeing 777, prompting recognition of their importance in lightweighting[1-3]. As a new generation of TiAl alloys, high Nb-TiAl alloys have higher service temperatures while maintaining light weight, which can meet the requirements of energy saving and emission reduction for the next generation of high-performance aero-engines[4, 5]. However, low-cost cast high-Nb-TiAl alloys have poor mechanical properties which limits their industrial applications. In this work, a research on simultaneously strengthening and toughening for high Nb-TiAl alloys by in-situ nanoscale silicides will be presented. This work was based on the theory of second-phase strengthening to achieve in-situ precipitation of high-density nanoscale silicides during the casting process by the addition of over-solubility silicon elements. Compared to the Ti-45Al-8Nb alloy, the Ti-45Al-8Nb-1.2Si alloy with a high density of nanoscale silicides had an increase in room-temperature tensile strength and total strain of 154% and 60%, respectively, as well as better mechanical properties at 800°C. Nanoscale silicides hindered the matrix dislocations moving and multiplying to strengthen and toughen the alloy was observed by transmission electron microscopy. In addition, the significant improvement in the high-temperature creep performance also originated from precipitated nanoscale silicides. By strengthening and toughening high-Nb-TiAl alloys with high-density nanoscale silicides, the thermal stability and service temperature will be enhanced.

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Advanced Dielectric Materials for Capacitors: Excellent Dielectric Performance in Germanium and Tantalum Co–Doped TiO2 Ceramics

Miss Yasumin Mingmuang[1], Narong Chanlek[2], Masaki Takesada[3], Pornjuk Srepusharawoot[1], Professor Prasit Thongbai[1]
[1]Khon Kaen University, Khon Kaen, Thailand, [2]Synchrotron Light Research Institute (Public Organization), Nakhon Ratchasima, Thailand, [3]Department of Physics, Hokkaido University, Sapporo, Japan

Session 3A: Alloys, ceramics and oxides, Auditorium, February 10, 2025, 16:35 - 17:55

Capacitors are energy storage devices characterized by high–power density, which is crucial for modern technological applications, particularly in electronic devices [1, 2]. In this study, the dielectric properties of materials, a key parameter for enhancing capacitors performance, were improved using simple oxide–based rutile TiO_2. The colossal relative permittivity ($\varepsilon'r>10^4$), associated with high capacitance (Cp~nF), can be easily achieved through doping with Ta5+. However, Ta5+ doping also results in a high dissipation factor (tanδ), leading to energy loss as heat. Notably, co–doping with Ge4+ and Ta5+ resulted in $\varepsilon'r$ ~$3.7–4.8\times10^4$ and significantly reduced tanδ to less than 0.05 at 1 kHz, while also improving the stability of ε'r across a wide temperature range, meeting the requirements for X8R ceramic capacitor types according to the Electronics Industries Alliance [3]. Moreover, the response of dielectric properties was tested under various operational conditions, including humidity and DC bias measurements. The presence of multivalence in Ti and oxygen loss in the lattice were detected on the surface of the polycrystalline ceramics, which consists of semiconducting grains surrounded by insulating grain boundaries. Experimental impedance spectroscopy analysis, combined with theoretical calculations using density functional theory (DFT), was employed to investigate the origins of the excellent performance in these Ge4+/Ta5+ co–doped rutile TiO_2 ceramics, attributing the results to a combination of intrinsic and extrinsic effects.

Keywords: Dielectric materials, Rutile TiO_2, Colossal permittivity, DFT, Impedance spectroscopy.

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The Effect of High-Energy Ball Milling on the Sintering Temperature Reduction in X7R-type Dielectric Material (Al0.5Nb0.5)xTi1-xO2.

Ms Jirata Prachamon[1], Mr. Prasit Thongbai[1,2]
[1]Giant Dielectric and Computational Design Research Group (GD–CDR), Department of Physics, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand, Khonkaen, Thailand, [2]Institute of Nanomaterials Research and Innovation for Energy (IN-RIE), NANOTEC-KKU RNN on Nanomaterials Research and Innovation for Energy, Khon Kaen University, Khon Kaen, 40002, Thailand, Khonkaen, Thailand

Session 3A: Alloys, ceramics and oxides, Auditorium, February 10, 2025, 16:35 - 17:55

This study explores the dielectric properties of (Al0.5Nb0.5)xTi1-xO2 ceramics, with doping levels of x = 0%, 2.5%, and 5%, synthesized using a high-energy ball milling technique to produce fine, uniform ceramic nanopowders.[1] The research focuses on how these properties, critical for applications in capacitors and insulators,[2] are influenced by varying doping levels and sintering processes. A key objective was to reduce the sintering temperature, with calcination performed at 1100 ºC for 2 h. X-ray diffraction (XRD) was employed to confirm the phase purity of TiO_2 in the ceramics. The nanopowders were further characterized using transmission electron microscopy (TEM), while the grain structure and elemental composition were analyzed using scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDX), respectively. The results revealed that ceramics sintered at 1200 ºC for 5 h exhibited a significant increase in dielectric permittivity, particularly at x = 2.5% (~29,000 at 1 kHz), which also demonstrated the lowest dielectric loss tangent (0.07). However, further increases in doping levels led to a decrease in dielectric permittivity. Additionally, impedance spectroscopy was used to investigate the electrical responses of grain boundaries and internal interfaces, providing further insights into the properties of materials.

Keywords: High energy ball mill, Dielectric properties, Impedance spectroscopy

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Ultrathin doped gallium oxide layers enabled by liquid metal alloys

Ms Laetitia Bardet[1], Ali Zavabeti[2], Amar Salih[3], Dawei Zhang[4], Mohammad Bagher Ghasemian[5], Yunlong Sun[4], Lucy Johnston[1], Danyang Wang[4], Jan Seidel[4], François Allioux[5], Cuong Ton-That[3], Kourosh Kalantar-Zadeh[5], Jianbo Tang[1]
[1]School of Chemical Engineering, University of New South Wales (UNSW), Sydney, Australia, [2]Department of Chemical Engineering, The University of Melbourne, Parkville, Australia, [3]School of Mathematical and Physical Sciences, University of Technology Sydney, Ultimo, Australia, [4]School of Materials Science and Engineering, UNSW, Sydney, Australia, [5]School of Chemical and Biomolecular Engineering, University of Sydney, Sydney, Australia

Session 3A: Alloys, ceramics and oxides, Auditorium, February 10, 2025, 16:35 - 17:55

The self-limiting oxidation of liquid metals in air forms an oxide layer a few nanometres thick which can be transferred to a large number of substrates. This provides a platform to fabricate 2D metal oxides and integrate them into novel electronic and optoelectronic systems. The incorporation of dopants into the liquid metal surface oxide is of both fundamental and technological significance, but this subject remains underexplored to date. Solute metals in a liquid metal solvent are found to behave differently when doping the surface-formed metal oxide.[1–4] In this work, we investigate the multi-element doping of the surface-formed liquid metal oxide layer of the eutectic gallium indium (EGaIn) liquid metal containing multiple dilute solvated elements. We dissolve gold, copper, palladium and platinum with the same nominal ratio (0.5 at%) in the parent EGaIn liquid metal.[5] This allows the exfoliation of a doped ultrathin oxide layer, predominantly composed of gallium oxide (Ga2O3). We show that the solute metals lead to different doping ratios in the Ga2O3 layer, depending on the temperature at which the oxidation/exfoliation takes place. This is thought to be a result of the solvent-solute interactions and energetics, rather than their relative abundance.[6] This work presents a novel doping approach at moderate temperatures to produce ultrathin doped Ga2O3 layers harvested from liquid metals, while preserving their high optical transparency.

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Doping Studies of Gallium Oxide Thin Films Produced Using Sol-Gel Techniques

Miss Kate Wislang[1,3], Dr Rodrigo Gazoni[2,3], Professor Roger Reeves[2,3], Professor Martin Allen[1,3]
[1]Electrical and Computer Engineering, University of Canterbury, Christchurch, New Zealand, [2]School of Physical and Chemical Sciences, University Of Canterbury, Christchurch, New Zealand, [3]MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand

Session 3A: Alloys, ceramics and oxides, Auditorium, February 10, 2025, 16:35 - 17:55

Ga_2O_3 is an ultra-wide bandgap semiconductor with a high thermal stability and breakdown strength, targeted for use in high-efficiency power electronics and solar-blind UV photodetectors [1]. Several common techniques to produce Ga_2O_3 exist; however, long growth times, low throughput, and high cost prevent Ga_2O_3 from reaching widespread adoption.

Using the Sol-Gel technique, transparent, smooth Ga_2O_3 thin films were produced at much faster growth rates and a fraction of the cost and energy demands. Economical Ga_2O_3 fabrication using Sol-Gel will change the landscape of electrical device manufacturing provided similar electrical properties can be achieved.

Sn- and Si-doped Sol-Gel Ga_2O_3 deposition on c-plane sapphire substrates was optimised to produce films of up to 500 nm thickness with 100% visible transparency and low surface roughness (0.3 nm rms). Both dopants showed significant Moss-Burstein type shifts in optical bandgap with doping concentration (maximum shift of 0.29 eV for Sn-doped material).

Electrical properties of 100 nm Sn- and Si-doped films were measured using Ti/Au Transmission Line Rings (TLR), with gap sizes of 10-75 µm, with the results indicating low dopant activation/mobility. Thicker 500 nm multi-layered films overcame surface depletion layer effects, increasing conductivity (10-6 A at 10 V, for 15 µm TLR gap size). Fabricated PtOx/Pt Schottky diode devices displayed strong rectifying behaviour [2].

Theoretical investigations suggest that F could be an effective donor in Ga_2O_3 [3]. Preliminary experimental results are encouraging; 200 nm 0.0005% SnF_2-doped Sol-Gel films produced a current of 10-5 A at 10 V, orders of magnitude higher than other dopants.

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Spectroscopy and modelling of oxygenated calcium fluoride doped with erbium and europium ions

Mr Michael Moull[1,2], Dr Jamin Martin[1,2], Ms Alice Jeffrey[3], Mr Timothy Newman[3], Dr John Bartholomew[3], Professor Jon-Paul Wells[1,2], Professor Michael Reid[1,2]
[1]University of Canterbury, Christchurch, New Zealand, [2]The Dodd-Walls Centre for Photonic and Quantum Technologies, New Zealand, [3]University of Sydney, Sydney, Australia

Session 3B: Photoactive materials and optical properties, Dobson 1, February 10, 2025, 16:35 - 17:55

Rare-earth doped materials are strong candidates for quantum information technologies that provide an interface between light and matter, such as quantum memories, repeaters and transducers. Coherent storage with a six-hour time-scale has been demonstrated in electron-nuclear hyperfine states of Europium ions in yttrium silicate [1]. Erbium is of particular interest due to it's compatibility with existing fibre-optic technologies [2]. A limitation of rare-earth optical technology is the low transition intensities between the 4f levels. Trigonal sites for rare-earth ions in CaF_2 may be created by oxygenation of the the crystals, where the substitution of an oxygen ion adjacent to the rare-earth ion gives extremely large dipole moments [3].

In this work we report spectroscopic studies of erbium and europium ions in oxygenated CaF_2. We demonstrate accurate modelling of the electronic and hyperfine energy level structure with a crystal-field model [4]. Crucially, we show that we can also model the optical transition intensities. Such detailed understanding of how the local environment affects the optical properties of rare-earth ions, combined with advanced fabrication techniques, has the potential to optimise performance for quantum technology applications.

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Controlling excited state localisation in molecular photosensitisers

Dr Georgina Shillito[1], Dr Stephan Kupfer[1], Prof Keith Gordon[2]
[1]Friedrich Schiller University Jena, Jena, Germany, [2]University of Otago, Dunedin, New Zealand

Session 3B: Photoactive materials and optical properties, Dobson 1, February 10, 2025, 16:35 - 17:55

The photophysical properties of a series of transition metal complexes, with potential light-harvesting and photocatalytic applications are explored in a joint synthetic, spectroscopic and theoretical investigation. [1-4]

A common drawback in the development of molecular photocatalysts is that the photoexcited states are not sufficiently long-lived to allow the catalytic mechanism to occur. [2] Herein we explore different means by which the excited state lifetime can be extended for a series of candidate structures. Thereby opening up possibilites for the development of long-lived excited state species, capable of both solar energy harvesting and generation of clean fuel, such a hydrogen.

The chemical and photophysical influence of different structural variations on the excited state deactivation pathways is investigated. The energetic order and character of the excited states is probed using a suite of methods, including steady-state resonance as well as time-resolved resonance Raman spectroscopy in conjugation with quantum chemical simulations.

We demonstrate that inclusion of secondary, organic donor groups, facilitate the population of long-lived intra-ligand charge transfer states. [1,3,4] Spin-orbit coupling calculations reveal that these organic-like states are not directly populated and instead are accessed via metal based gateways.

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Photoactive 3d transition metal complexes

Dr Stephan Kupfer[1]
[1]Friedrich Schiller University Jena, Jena, Germany

Session 3B: Photoactive materials and optical properties, Dobson 1, February 10, 2025, 16:35 - 17:55

Solar energy conversion is among the most promising approaches to transform our energy sector towards sustainability. In this context, photocatalysis allows the conversion of sunlight into chemical energy such as molecular hydrogen. Typically, both the light-harvesting unit as well as the catalytic centres in (supra)molecular photocatalysts heavily rely on precious 4d and 5d transition metals due to their favourable photophysical and electrochemical properties, alongside thermal, light and pH stability. Thus, the broadscale application of such systems is limited by the scare availability of these metals.

Unfortunately, utilizing earth-abundant 3d metal-based photosensitizers, e.g. Fe(II) complexes, suffers from excited-state lifetimes in the ps regime limiting the photocatalytic ability.[1,2]

Here, we investigate the photophysical and photochemical properties of a series of $3d^6$ transition metal complexes and derive detailed insight regarding structure-property relationships.[3] Thereby, we focus on the redox-active charge transfer states which are of particular interest in the frame of photocatalysis as well as on the accessibility of prominent – yet undesirable – excited-state deactivation channels via the so-called metal-centred states. Based on the computational modelling using state-of-the-art multiconfigurational methods and cost-efficient (scalar-relativistic) time-dependent density functional theory in association with time-resolved spectroscopy, we present selected aspects of our theory-driven design concepts to drive the desired electron and energy transfer processes,[3] 2nd coordination sphere effects[4] as well as self-healing strategies[5] to enhance the photostability of earth-abundant transition metal complexes. Finally, we focus on simulating competitive intermolecular electron transfer processes in preassembled, e.g., by π-stacking, photoactive dyads in the frame of CO_2 reduction.[6]

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Raman studies of triphenylamine-based acceptor-donor dyes

Miss Elkhansa Elbashier[1], Prof Keith Gordon[1], Prof Pawel Wagner[2]
[1]Department of Chemistry, University of Otago, Dunedin 9016, New Zealand, [2]Australian Institute of Innovative Materials, University of Wollongong, Wollongong, Australia

Session 3B: Photoactive materials and optical properties, Dobson 1, February 10, 2025, 16:35 - 17:55

Three organic donor-acceptor dyes, each with a triphenyl donor and varying acceptor functional groups, were studied to explore the impact of functional group substitution on their photochemical properties. The dyes investigated include TPA-π-InCN2 (two malononitrile groups), TPA-π-InO2 (two ketone groups), and TPA-π-InOCN (mixed functional groups). Spectroscopic techniques, including Raman spectroscopy, UV-vis absorption, and emission spectroscopy, complemented by density functional theory (DFT) calculations, were used to characterize these dyes. Theoretical calculations provided insights into electronic structure and molecular vibrations. Shifts in Raman spectra between solid-state and solvent-state samples revealed that solvation significantly alters ground-state polarity. Resonance Raman spectroscopy identified three distinct electronic transitions in the UV-vis spectra: a high-energy π-π* transition and two charge transfer (CT) transitions. DFT and experimental analyses indicated that absorption bands in the 491–591 nm range in dichloromethane (DCM) are attributed to twisted intramolecular charge transfer (TICT). The malononitrile group caused a red-shifted absorption band and a more bent ground-state geometry, leading to TPA-π-InCN2 having the highest nonradiative decay and lowest quantum yield. The presence of two distinct functional groups in TPA-π-InOCN generated two accepting orbitals with different energies, contributing to its higher molar absorptivity and quantum yield (0.25). Lifetimes for these dyes were around 5 ns, with the ketone group increasing the lifetime. The Lippert-Mataga analysis, conducted using seven solvents, indicated the highest dipole moment change (28.9 D) for TPA-π-InOCN.

Plasma-Assisted Printing of Antimicrobials Set to Replace Industry Standards.

Mr Daniel Carleton[1]
[1]Auckland University of Technology, Auckland, New Zealand

Session 3C: Antimicrobial materials, Dobson 2, February 10, 2025, 16:35 - 17:55

The pandemic made us all cognisant of the importance of antimicrobial agents in combatting microorganisms. While a plethora of products are available for surface disinfection, most are incompatible with the human body. Antimicrobial peptides, applied using an Atmospheric Pressure Plasma Jet, offer a novel, biocompatible coating which overcomes the various problems of the existing technology.

Our technology introduces a fine mist of antimicrobial agent, into a jet of cold plasma, and deposits the material onto practically any desired substrate. In many cases, the plasma even changes the surface chemistry of the substrate allowing the material to bond with a greater strength than through traditional application methods.

This technology offers a low-temperature, low-solvent, fast coating application. This makes it ideal for flexible materials like catheters or any electrical component that cannot handle the high heat of an autoclave. It also provides a biocompatible coating to medical implants, such as hip replacements or pacemakers, to lower the risk of rejection.

Our results also show that the coating outperforms the leading existing technology in antimicrobial efficacy, coating speed, as well as coating resilience. We believe that such technology could revolutionise the medical industry and significantly reduce the rate of infection during surgeries.

Accelerating Lab- to- Bedside Biodegradable Nanomaterial- based Antimicrobial Innovation

Dr Shreehari Kodakkat[1], Dr Aaron Elbourne[2], Professor Sumeet Walia[3], Dr Saffron Bryant[4]
[1]RMIT University, Melbourne, Australia, [2]RMIT University, Melbourne, Australia, [3]RMIT University, Melbourne, Australia, [4]RMIT University, Melbourne, Australia

Session 3C: Antimicrobial materials, Dobson 2, February 10, 2025, 16:35 - 17:55

Antimicrobial resistance (AMR) is a growing global health crisis that threatens to undermine decades of medical progress, with current antibiotics becoming increasingly ineffective against resistant pathogens.

Exacerbating this issue is the significant reduction in the development of new antibiotics, requiring innovative approaches to combat these threats. My research aims to accelerate the translation of lab-based antimicrobial biodegradable nanomaterials into clinical applications, addressing this urgent need.

The project is structured into three phases. The first phase focuses on determining the antimicrobial efficacy of biodegradable nanomaterials. This involves screening and in vitro studies to identify materials that effectively combat multidrug-resistant microbes while maintaining biocompatibility. The second phase delves into the mechanisms of action of these nanomaterials. This includes studying the degradation of nanomaterial flakes and the generation of reactive oxygen species (ROS), as well as their interactions with cell membranes, which collectively contribute to their antimicrobial properties.

The final phase of the project involves ADME (Absorption, Distribution, Metabolism, and Excretion) studies to optimize drug delivery. Here, we focus on enhancing the delivery and efficacy of these nanomaterials using Eutectogels, which provide a sustained release mechanism and improved bioavailability.

This comprehensive approach not only aims to develop effective antimicrobial agents but also seeks to bridge the gap between laboratory research and bedside application, offering a promising strategy to tackle the escalating challenge of antimicrobial resistance.

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Development of Bactericidal Nanostructures on 3D Polymeric Surfaces

Mr Buddhika Sampath Kumara Sinhasana Pattale Siriwedi Naidelage[1,2,3], Dr. Amal Senevirathne[1,3], Dr. Asha Mathew[1,5], Ms. Preetha Ebenezer[1,3], Dr. Laura Bray[1,3], Prof. Prasad K.D.V Yarlagadda[1,2,3,5], Dr. Mohammad Mirkhalaf[1,3,4]

[1]School of Mechanical, Medical and Process Engineering, Faculty of Engineering, Queensland University of Technology (QUT), Brisbane, Australia, [2]Australian Research Council Training Centre for Multiscale 3D Imaging, Modelling, and Manufacturing, Queensland University of Technology (QUT), Brisbane, Australia, [3]Centre for Biomedical Technologies, Queensland University of Technology (QUT), Brisbane, Australia, [4]Centre for Materials Science, Queensland University of Technology (QUT), Brisbane, Australia, [5]School of Engineering, University of Southern Queensland, Springfield, Australia

Session 3C: Antimicrobial materials, Dobson 2, February 10, 2025, 16:35 - 17:55

Biomedical implant and device failures resulting from bacterial infections constitute a significant issue in the field of biomedicine, leading to antibiotic resistance, increased healthcare costs, morbidity, and mortality [1]. The developments of artificial antibacterial nanostructured surfaces inspired by natural antibacterial surfaces, such as cicada and dragonfly wings, have been initiated [2], [3]. Most of these artificial surfaces have been produced on metals and ceramics through complex, non-facile processes [1], [4]. However, these methods are generally effective only on 2D external surfaces, which are not representative of the actual implants and devices used in clinical practice. These implants and devices typically have complex internal and external geometries. Despite the numerous advantages that polymers offer, such as light weight, anti-corrosion properties, 3D printability, biocompatibility, and biodegradability, there is currently no method for creating bactericidal nano-surfaces on 3D internal and external surfaces of polymers. This study aims to develop a bactericidal nanostructured surface on polylactic acid (PLA) polymer by modifying the conventional hydrothermal synthesis process, which is typically used to fabricate bactericidal nanostructures on titanium and its alloys [1], [2]. This modification can effectively create different nanostructures at low temperature conditions on both the internal and external surfaces of the polymer. The surface nano-features was assessed using scanning electron microscopy (SEM), atomic force microscopy, and drop shape analysis. The surface chemistry was assessed via fourier-transform infrared spectroscopy and SEM-energy dispersive spectroscopy. Bactericidal efficacy was assessed via LIVE/DEAD™ BacLight™ bacterial viability kits for both Pseudomonas aeruginosa (Gram-negative) and Staphylococcus aureus (Gram-positive) bacteria species.

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Active surface coatings with intrinsic antimicrobial properties

Mrs Sandya Athukoralalage[1], Dr Keng Chew[2], Dr Nasim Amiralian[1]
[1]Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, St Lucia 4072, Australia, [2]School of Chemistry and Molecular Biosciences, The University of Queensland, St Lucia 4072, Australia

Session 3C: Antimicrobial materials, Dobson 2, February 10, 2025, 16:35 - 17:55

The recent surge in pandemic outbreaks has underscored the critical need for innovative approaches to reduce pathogen transmission through contaminated surfaces. Current surface sanitation technologies, despite their potential, struggle with challenges related to scalability, environmental impact, and versatility. In this work, the development and evaluation of a sustainable functional surface coating that combines intrinsic antimicrobial and low fouling properties will be explored. A porous, reactive cellulose fibre network with dialdehyde functionality was developed, exhibiting strong antiviral and antibacterial activity against Staphylococcus aureus, Escherichia coli, and the influenza A/H1N1 virus. In addition, it will be demonstrated how the wettability of this coating significantly reduces bacterial adhesion and colony formation, including the elimination of dead debris. The biocompatibility of the active cellulose fibres was assessed, revealing no acute toxicity in L929 cells, ensuring the coating's safe application on contact surfaces. Sustainability will be emphasised, as the coating leverages dialdehyde cellulose derived from agricultural waste, reducing reliance on toxic chemicals and promoting circular economy principles. Potential applications of this sustainable, cost-effective, and scalable material across various sectors, including medical facilities, public infrastructure, packaging, and household products will be discussed. This work contributes to advancing more effective and environmentally friendly infection control solutions.

Materials Characterisation and Modelling, Critical for the Materials Development Lifecycle

Ms Jacinta White, Mrs Natasha Wright[1], Dr Roger Mulder, Dr Sherry Mayo
[1]Csiro, Clayton, Victoria, Australia

Session 3D: Materials characterisation, porous and functional materials, Dobson 3, February 10, 2025, 16:35 - 17:55

Materials Characterisation and Modelling are integral to the materials development lifecycle, providing the evidence, data and insights which underpin every step of this complex process. Characterisation of Novel Materials can be a significant challenge due to the complex systems and interfacial interactions of the constituents, which can be at levels ranging from subnano - to micro-scale. Compared with conventional, bulk analyses, the need for the ability to holistically characterise the distributions and interactions has continued to grow in importance within CSIRO. In this paper the application of ultra-high resolution imaging (including 3D tomography), micro and thin film X-ray diffraction, spectroscopic and various surface analysis techniques (XPS, AFM) have been employed to holistically characterise several examples of custom engineered novel materials developed by CSIRO's Manufacturing Research Unit.

Crystal Engineering of Hybrid Framework Materials Incorporating a Tantalum Based Pillar

Dr Nathan Harvey-Reid[1,2,3], Dr. Debobroto Sensharma[4], Dr Soumya Mukherjee[4], Dr. Komal Patil[1,3], Dr. Shi-Qiang Wang[4], Professor Michael Zaworotko[4], Professor Paul Kruger[1,3]
[1]University of Canterbury, Christchurch, New Zealand, [2]Paihau-Robinson Research Institute, Victoria University of Wellington, Wellington, New Zealand, [3]MacDiarmid Insitute for Advanced Materials and Nanotechnology, Wellington, New Zealand, [4]Bernal Institute, University of Limerick, Limerick, Republic of Ireland

Session 3D: Materials characterisation, porous and functional materials, Dobson 3, February 10, 2025, 16:35 - 17:55

Hybrid framework materials can be defined as a sub class of porous materials such as metal-organic frameworks (MOFs) that contain inorganic pillaring units in their structure. These scaffolds take advantage of ultramicroporous channels (<7 Å) and highly fluorinated pillars (SiF_6,TiF_6,etc.) to provide strong binding interactions with guest molecules within the framework pores. Thanks to such characteristics, a handful of these materials have shown exceptional selective capture and separation for numerous small polarisable gases (eg. C_2H_2/CO_2, C_2H_2/C_2H_4, CO_2/N_2).

Herein is reported a series of novel hybrid frameworks, derived from the recently reported $TaOF_5$ pillar to provide further insight into how different pillars affect this platform. Along with the $TaOF_5$ pillar, two different organic ligands and metal nodes were used, to yield a total of four novel framework materials. This study also identified that $TaOF_5$ arose via the hydrolysis of TaF_7 in situ.

Each framework was characterised with a range of techniques and through pure gas adsorption experiments to assess the effect the $TaOF_5$ pillar and different ligand and metal node combinations have upon each framework's sorption performance. One of the new materials, was found to be a good candidate for a variety of gas separation processes.

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Multicomponent Metal-Organic Frameworks Using Amino Acid and Peptide Ligands

Mrs Ghadir Dahalan[1]
[1]Massey University, Palmerston North, New Zealand

Session 3D: Materials characterisation, porous and functional materials, Dobson 3, February 10, 2025, 16:35 - 17:55

Multicomponent metal-organic frameworks (MMOFs) are a type of MOFs that consist of multiple structurally unique ligands and/or metal ions/clusters. There has been an interest in flexible ligands such as amino acids and peptides.[1-4] However, all studies to date have used one kind of ligand. We present the first multicomponent amino acids MOFs using combinations of amino acids as ligands.

The Telfer Group has consistently focused on MMOFs since the unveiling and documenting MUF-7 and MUF-77 (MUF = Massey University Framework). [5, 6] Amino acids have been incorporated into the conventional MUF-77 ligands, where the amino acid acts as a side arm. A key application of this approach revolves around catalysis. The most potent catalysts are enzymes, that leverage their catalytic effectiveness from the precise arrangement of functional groups within the active site, coupled with a degree of dynamic and flexible behaviour. The pores within the multicomponent frameworks (MUF-77) are anticipated to offer analogous reaction environments suitable for catalysis. Through the incorporation of multiple amino acids into the framework, the pores may loosely resemble enzyme-active sites.[7, 8]

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Next-generation zeolite oxygen concentrator: a lifecare solution for COPD patients

Ms Christina Howat[1], Prof Alex C. K. Yip[1]
[1]University of Canterbury, Christchurch, New Zealand

Session 3D: Materials characterisation, porous and functional materials, Dobson 3, February 10, 2025, 16:35 - 17:55

Chronic obstructive pulmonary disease (COPD) is the third leading cause of death worldwide.[1] In Aotearoa alone, 200,000 individuals live with COPD, with Māori and Pasifika communities disproportionately affected.[2] To alleviate symptoms of COPD, portable zeolite oxygen concentrators are the most promising lifecare solution. Current portable zeolite oxygen concentrators are expensive (>NZ$5,500) and short-lived because of demanding pressure swing adsorption technology.[3] High-pressure conditions are necessary for current zeolite beds to adsorb nitrogen from air to produce a concentrated oxygen stream.[4] The cycling of high-pressure conditions is energy demanding and with continued use, will deteriorate the zeolite bed. Used zeolite beds are rarely regenerated and are hard to replace. Therefore, a new zeolite with selectivity for nitrogen at milder pressure conditions is needed for an affordable, efficient, and sustainable portable oxygen concentrator. Here, we propose a novel high-density multivalent cation-exchanged zeolite X, capable of selective adsorption of nitrogen at lower pressures. A synthetic strategy involving successive ion-exchange reactions will be used to create a new combination of multivalent cations in zeolite X. The proposed combination of multivalent cations is predicted to show high selectivity for nitrogen at lower pressures by manipulation of electrostatic interactions in the zeolite. This next-generation zeolite X can support aspects of social, economic and environmental sustainability in Aotearoa. Moreover, it can extend to industrial oxygen applications and reduce the need for cryogenically distilled oxygen.

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Analysis of pyrolysis reactions for tris(dialkylamino)cyclopropenium chloride salts

Mr Askin Eldiven[1], Assoc Prof Owen Curnow[1], Prof Aaron Marshall[2], Dr Nic Bason[3]
[1]School of Physical and Chemical Sciences, University of Canterbury, Christchurch, New Zealand, [2]School of Physical and Chemical Sciences, University of Canterbury, Christchurch, New Zealand, [3]Syft Technologies Limited, Christchurch, New Zealand

Session 3D: Materials characterisation, porous and functional materials, Dobson 3, February 10, 2025, 16:35 - 17:55

There is a growing interest in the production of nitrogen-doped carbon materials due to their excellent carbon-enhancing properties. Such as in conductivity, basicity, oxidation stability, catalytic activity, cycle performance, and increased wettability, [1] showing improvements in electrochemical applications. [2] [3]

Among various precursor options, imidazolium- and pyridinium-based ILs have emerged as notable candidates for producing functional carbon-based nanomaterials. [4] [5] This study focuses on investigating the thermal stability of cyclopropenium-based ILs by analysing the pyrolysis mechanisms of the chloride salts and their subsequent carbonization, producing nitrogen-doped carbon materials. By coupling a thermogravimetric analyzer with residual gas analyzer (TGA-RGA), supported by techniques such as microanalysis, differential scanning calorimetry (DSC), selected ion flow tube mass spectrometry (SIFT-MS), and scanning electron microscopy-energy dispersive X-ray spectroscopy (SEM-EDX) data, we investigate the kinetic properties of the IL before and during their polycondensation reaction. This investigation tracks the volatile gas production during the pyrolysis reaction. Particularly, $[C_3(NEt_2)_3]Cl$ demonstrates a distinctive reaction mechanism, underscoring its unique and promising characteristics in our research context.

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Multipole order and chirality in solids

Professor Uli Zuelicke[1], Roland Winkler[2,3]
[1]Victoria University of Wellington, Wellington, New Zealand, [2]Northern Illinois University, DeKalb, USA, [3]Argonne National Laboratory, Lemont, USA

Session 3E: Condensed matter and magnetic materials, Dobson 4, February 10, 2025, 16:35 - 17:55

Electric and magnetic order in solids is the basis of modern electronics; but it is also the foundation of future technologies in magnetoelectronics and spintronics. Remarkably, a systematic theory of electric and magnetic order in crystals has been missing so far. Here we present such a theory [1,2], and we show how the electric and magnetic order shapes the electronic band structure that is directly relevant for many applications. We identify two complementary, comprehensive classifications of crystals, based on five categories of electric and magnetic multipole order (parapolar, electropolar, magnetopolar, antimagnetopolar, and multipolar) and five categories of chirality (parachiral, electrochiral, magnetochiral, antimagnetochiral, and multichiral). Each category of chirality arises from distinct superpositions of electric and magnetic multipole densities. We provide a complete theory of minimal effective models characterizing the different categories of chirality in different systems. Jointly these two schemes yield a classification of all 122 magnetic crystallographic point groups into 15 types that treat space inversion, time inversion and their combined inversion on the same footing.

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Anisotropic Magnetoresistance and the Fermi surface of GdN

Mr Ted Trewick[1,2], Prof. Ben Ruck[1,2], Dr. William Holmes-Hewett[2,3], Prof. Joe Trodahl[1]
[1]School of Chemical and Physical Sciences, Victoria University of Wellington, P.O. Box 600, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, P.O. Box 600, New Zealand, [3]Robinson Research Institute, Victoria University of Wellington, P.O. Box 33436, New Zealand

Session 3E: Condensed matter and magnetic materials, Dobson 4, February 10, 2025, 16:35 - 17:55

The lanthanide nitrides (LnN) are a series of intrinsic ferromagnetic semiconductors and as such are the subject of increasing interest in both fundamental and applied fields [1]. The successful application of this rare confluence of electronic and magnetic ground states requires a full understanding of both. Gadolinium Nitride, the central member of the series, provides a clear starting point, and significant effort has been placed into understanding its properties thus far [2,3,4,5].

While the electron wavefunctions and thus the properties of the LnN can be calculated using Density Functional Theory (DFT), there are many predictions which lack experimental validation, particularly those relating to electron transport.

Here we provide an experimental link between calculations and the physical material, showing that the shape of the Fermi surface of Gadolinium Nitride closely matches that predicted from DFT. In particular we find that the magnetoconductivity tensor, derived using the Boltzmann transport equation in the relaxation time approximation on the electron wavefunctions taken from DFT calculations, reproduces the structure and field dependence of the experimentally measured anisotropic magnetoresistance (AMR). This correspondence validates the computational work and motivates the use of parameters derived from the band structure in the design of realistic devices.

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Engineering of emergent magnetism in functional oxide superlattices

Dr Freddy Lyzwa[1,2], Prof. Dr. Vasily Moshnyaga[3]
[1]The University of Auckland, Auckland, New Zealand, [2]Te Whai Ao The Dodd-Walls Centre for Photonic and Quantum Technologies, New Zealand, [3]Erstes Physikalisches Institut, University of Göttingen, Friedrich-Hund-Platz 1 37077, Göttingen, Germany

Session 3E: Condensed matter and magnetic materials, Dobson 4, February 10, 2025, 16:35 - 17:55

Relatively low transition temperatures and formation of extended defects at interfaces are the two main drawbacks hindering functional manganite structures to be used in the next generation electronic devices.

We address both aspects by comprehensive structural, optical and magneto-electric studies of epitaxial (LaMnO3)m/(SrMnO3)n/SrTiO3 superlattices (SLs) prepared in a wide range of growth parameters using a metalorganic aerosol deposition (MAD) [1]. A novel emergent ferromagnetic phase with high TC=360 K is shown to result from a charge transfer at the atomically sharp interfaces [2]. The length scale of the charge transfer and emerging magnetism is shown to be controlled through the “m/n” thickness ratio [3].

Recently, a modified MAD has been developed and applied for the growth of SLs with “gradient” interfaces, where LaMnO3 changes to SrMnO3 on the length scale D = 0 - 10 u.c.. Remarkably, a complex two-phase magnetic behavior was observed for most gradient SLs with TC increasing for higher D. We discuss the new findings in terms of atomic (chemical) and electronic intermixing, and propose new perspectives on effective interface engineering in functional oxide heterostructures.

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Controlling Skyrmions in Cu2OSeO3 through Doping: Insights into the Relationship Between Crystal Structure and Magnetic Ordering

Mr Marco Vas, Professor Tilo Söhnel[1,2], Dr Samuel Yick[1,2], Mr Alexander Ferguson[1,2], Eda Vella[1,2], Professor Elliot Gilbert[3], A/Prof Clemens Ulrich[4]

[1]University of Auckland, Auckland, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand, [3]Australian Centre for Neutron Scattering, ANSTO, Lucas Heights, Australia, [4]University of New South Wales, Sydney, Australia

Session 3E: Condensed matter and magnetic materials, Dobson 4, February 10, 2025, 16:35 - 17:55

Magnetic Skyrmion lattices (SkL) are spin ordering which are topologically protected due to their quantised winding number. This, along with other helimagnetic orderings offer a plethora of fascinating phenomena for fundamental research and applications.[1] Cu2OSeO3 is an insulating multiferroic material that has shown to host SkL at specific conditions.[2] It possesses a magnetic structure with both ferromagnetic (FM) and antiferromagnetic (AFM) superexchange interactions being present and has a 3-up 1-down ferrimagnetic arrangement of Cu2+ ions.[3] The lack of inversion symmetry in the corner shared O-Cu4 tetrahedra lattice results in an appreciable DMI between Cu2+ sites; this competes with FM/AFM interactions leading to spin canting formation of helical/conical spin textures at different fields and temperature conditions.[2] Due to the absence of a crystallographic transformation throughout the temperature range alongside the formation of the magnetic phases, it has been commonly assumed that the structure plays a passive role in magnetic ordering.[3]

Yet, published studies have challenged this assumption, which shows that internal expansion leads to a decrease in Tc for the helical to paramagnetic transition.[4] Furthermore, observation by Nishibori et al. shows that by applying pressure, Tc increases as the unit cell volume contracts.[5]

In this work, we incorporated both magnetic and non-magnetic ions into the Cu2OSeO3 host. The inclusion of Te into the Se-sites and Co into the Cu-sites changed the crystal and magnetic structure, respectively. The skyrmion dynamics and spin interactions within these materials were then studied using synchrotron X-ray powder diffraction, neutron powder diffraction, and magnetometry.

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Dimensionality-driven novel properties of topological semimetals and applications

Professor Suk-Ho Choi[1]
[1]Kyung Hee University, Yongin, South Korea

Session 3E: Condensed matter and magnetic materials, Dobson 4, February 10, 2025, 16:35 - 17:55

Integrating low-dimensional materials have widened the spectrum of building blocks for creating hybrid heterostructure systems with unique functionalities and excellent performance [1-3]. The intriguing electronic structure of topological semimetals (TSMs), representing a novel class of condensed matter, is of fundamental interest because of their exotic quantum nature and potential for next-generation device applications such as high-speed electronics, spintronics, and quantum computations. In this talk, I discuss our recent findings on a Dirac- to Weyl-semimetal (WSM) phase transition in Dirac semimetal Bi0.96Sb0.04 single crystals by Au-ion implantation and 2D WSM states achieved by a thickness-dependent topological phase transition of Bi0.96Sb0.04 thin films, thereby exhibiting novel transport of charge carriers.

Dimensionality- and topology-driven metal-insulator transition behaviors accompanied by abrupt variations of carrier type/density in the thin films are discussed based on the theoretical calculations. The photogalvanic effect of the inversion-symmetry-broken WSM states is studied for their possible energy harvesting applications.

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Conducting polymer devices to study the gut-brain axis

Róisín Owens[1]
[1]University of Cambridge, Cambridge, United Kingdom

Plenary Session 3, Auditorium, February 11, 2025, 08:30 - 09:30

The gut microbiome plays a vital role in human health and disease, particularly through the gut-brain axis, which is the communication axis between the gastrointestinal (GI) tract and the nervous system. This connection involves the vagus nerve, the immune system, and metabolites produced by gut bacteria. The microbiome-gut-brain axis (MGBA), has emerged as an incredibly important, but complex, part of human physiology. Dysregulation or disruption of the MGBA is implicated in a host of pathologies that affect brain and gut (e.g. Autism Spectrum disorder, Crohn’s disease) but also whole body disorders where inflammation and metabolism are affected (e.g. diabetes). Physiologically relevant in vitro human models, as well as advanced tools to study in vivo animal models, are urgently required to elucidate mechanisms in MGBA. Until recently, the majority of studies that seek to explore the mechanisms underlying the microbiome-gut-brain axis relied almost exclusively on animal models. Despite the great progress made with these models, various limitations, including ethical considerations and interspecies differences that limit the translatability of data to human systems, pushed researchers to seek for alternatives.

Physiologically relevant in vitro human models, as well as advanced tools to study in vivo animal models, are urgently required. In this talk I’ll discuss a new generation of electronic tools, based on conducting polymers, for understanding the gut-brain-microbiome axis. First, I’ll discuss our progress towards generating a complete platform of the human microbiota-gut-brain axis with integrated monitoring and sensing capabilities. Bringing together principles of materials science, tissue engineering, 3D cell biology and bioelectronics, we are building advanced models of the GI, with integrated real-time and label-free electronic monitoring, aiming to elucidate the role of microbiota in the gut-brain axis communication.

Second, I’ll discuss conformable electronic devices we’ve developed for both ex-situ measurements of GI tissue from rats, as well as in vivo experiments in live rats. These devices allow highly sensitive monitoring of impedance of the tissue (as an indicator of gut health) as well as the enteric nervous system.

Electrochemistry in Small Droplets

Dr Minkyung Kang[1]
[1]The University of Sydney, Camperdown, Australia

Keynote Session 6, Auditorium, February 11, 2025, 09:35 - 10:10

The investigation of electrochemical processes within droplets provides a unique opportunity to explore phenomena at or below the microscale, revealing insights that are frequently overlooked in bulk measurements. This study emphasises the importance of measuring and characterising electrochemical phenomena in small-scale environments, illustrating how this approach advances the understanding of local electrochemical behaviour and its implications for diverse applications.

One of electrochemical techniques, facilitating such detailed analysis, is scanning electrochemical cell microscopy (SECCM). SECCM has the advantage of probing local electrochemical processes with high spatial and temporal resolution, facilitating the integration of electrochemical data with structural and chemical information through correlative electrochemical multimicroscopy approaches. This capability is essential for material functional characterisation, as it correlates the electrochemical performance of materials with their structural and chemical properties. The application of SECCM is further extended to the study of phase transition reactions, herein, particularly the transition from liquid to gas (e.g., water to hydrogen), within confined droplet volumes. In these constrained environments, mass transport of gas is significantly influenced by the three-phase boundaries (electrode/electrolyte/air), which are crucial for understanding various applications, including bubble dynamics in metal processing and electrolysis. This study demonstrates how SECCM can be utilised to modulate bubble nucleation and dissolution within such confined volumes, providing novel insights into the interplay among electrochemical processes, surface chemistry, and phase transitions.

Information Processing in Dopant Network Processing Units

Professor Wilfred G. van der Wiel[1,2]
[1]BRAINS - University of Twente, Enschede, Netherlands, [2]University of Münster, Münster, Germany

Keynote Session 7, Dobson 4, February 11, 2025, 09:35 - 10:10

Throughout history, humans have harnessed matter to perform tasks beyond their biological limits. Initially, tools relied solely on shape and structure for functionality. We progressed to responsive matter that reacts to external stimuli and are now challenged by adaptive matter, which could alter its response based on environ-mental conditions. A major scientific goal is creating matter that can learn, where behavior depends on both the present and its history. This matter would have long-term memory, enabling autonomous interaction with its environment and self-regulation of actions. We may call such matter 'intelligent' [1,2].

Here we introduce a number of experiments towards 'intelligent' disordered nanomaterial systems, where we make use of 'material learning' to realize functionality. We have earlier shown that a 'designless' network of gold nanoparticles can be configured into Boolean logic gates using artificial evolution [3]. We later demon-strated that this principle is generic and can be transferred to other material systems. By exploiting the nonlinearity of a nanoscale network of dopants in silicon, referred to as a dopant network processing unit (DNPU), we can significantly facilitate handwritten digit classification [4]. An alternative material-learning approach is followed by first mapping our DNPU on a deep-neural-network model, which allows for applying standard machine-learning techniques in finding functionality [5]. Multi-DNPU networks can solve more complex tasks than individual DNPUs [6,7]. Finally, we show that our devices are not only suitable for solving static problems but can also be applied in highly efficient real-time processing of temporal signals at room temperature [8].

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Development of Sustainable Electrocatalysts for Anion Exchange Membrane Fuel Cells

Dr Hamish Andrew Miller[1], Dr Marco Bellini, Dr Maria Pagliaro, Dr Tailor Peruzzolo, Ms Carolina Castello, Dr Francesco Bartoli
[1]Consiglio Nazionale Delle Ricerche, Florence, Italy

Session 4A: Electrocatalysis, Auditorium, February 11, 2025, 10:40 - 12:45

In 2016, for the first time a polymer electrolyte fuel cell with no Pt based electrocatalysts delivered more than 0.5 W cm-2 of peak power density from H2 and air (CO2 free).[1] This was achieved with an Ag oxygen reduction (ORR) cathode and a Pd-CeO2 hydrogen oxidation reaction (HOR) anode electrocatalyst. The hydrogen oxidation (HOR) reaction under alkaline conditions is a kinetically slow process even when Pt group metals are employed. Our strategy to improve the alkaline HOR activity of transition metal nanoparticles is through engineering strong interactions with transition-metal oxides incorporated in carbon based catalyst supports.[2] Peak power densities of up to 2 W cm-2 were obtained when Pd-CeO2 is incorporated in AEMFC testing.[3] Regarding liquid e-fuels we are currently developing a 100 W fuel cell system using anion exchange membranes and non-Pt catalysts. The fuel cell stack will be fed with aqueous solutions of potassium formate produced from renewable energy and CO2. This work is funded by the EU Horizon Europe (Project FRESH - GA 101069605) [4].

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Repurposing Li ion battery materials as electrocatalysts for water splitting

Professor Anthony O'Mullane[1], Ms Arshdeep Kaur[1]
[1]Queensland University of Technology, Brisbane, Australia

Session 4A: Electrocatalysis, Auditorium, February 11, 2025, 10:40 - 12:45

Electrochemical reactions are at the heart of established and emerging technologies that will play a critical role in the green energy transition away from fossil fuels. This will involve the development of cheap catalysts for green hydrogen production but also the use of batteries for the electrification of industry and the transport sector. However, given the ubiquitous nature of Li ion batteries and their continued increase in usage, there is an emerging waste issue at their end of life [1]. This can lead to significant environmental problems if not dealt with correctly, however it also opens up an opportunity to use these battery materials in a new way [2].

In this talk I will describe our recent efforts to recycle spent Li ion batteries and repurpose the active materials into electrocatalysts that are suitable for electrochemical water splitting. Specifically, I will show how the current collector [3] and Li ion cathode materials such as Ni, Mn, Co (NMC) oxide and lithium iron phosphate can be developed into efficient and robust electrocatalysts for water splitting reactions. The impact of battery history on electrocatalytic performance will also be discussed.

This concept of urban mining may relieve pressure on existing resources while also protecting the environment from harmful waste.

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Investigating the use of Plasma Thermal Spraying for Alkaline Water Electrolysis Electrode Fabrication

Mr Glen McClea[1,2], Professor Aaron Marshall[1,2], Associate Professor Steve Matthews[1,3]
[1]University Of Canterbury, Christchurch, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, New Zealand, [3]University of Auckland, Auckland, New Zealand

Session 4A: Electrocatalysis, Auditorium, February 11, 2025, 10:40 - 12:45

To establish the wide-scale adoption of low-carbon hydrogen via water electrolysis, reducing the levelized cost of hydrogen through high-performing electrocatalysts is necessary [1]. Alkaline-based water electrolysis has seen a recent resurgence in research and development, due to the growing concern over the reliance on platinum group metals as electrocatalysts in acidic conditions [2].

Traditionally used to deposit protective coatings, plasma thermal spraying has recently gained attention as a large-scale electrode manufacturing technique. In this process, a catalyst powder is fed into the plasma plume of the plasma torch. Within the high-temperature, high-velocity plume the powder particles are melted and accelerated toward the substrate, where they collide to form a catalyst-coating layer upon impact [3]. This low catalyst loading leads to a reduced capital cost. With versatile feed material and operating conditions, this method offers high tunability and is suitable for fabricating large surface area electrodes [4].

In this study, the scale-up feasibility of plasma-sprayed electrocatalysts for alkaline water electrolysis was investigated. The electrodes were first characterized using scanning electron microscopy and X-ray diffraction. The electrochemical performance of the electrodes was analysed using a three-electrode cell with a 1 cm² active surface area, revealing high activity towards both the oxygen and hydrogen evolution reaction. To replicate industrial conditions, the electrodes were then tested in a 25 cm² two-electrode cell in 30 wt.% KOH at 60 ⁰C, achieving a stable cell current of 10 A. This initial success leads toward an industrial-scale proof-of-concept for plasma-sprayed electrodes.

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Mapping Location of Oxygen Nanobubble Formation on Nickel Surfaces

Miss Rizki Putri Andarini[1], Emily Wong[1], Dr Kim McKelvey[1]
[1]Victoria University of Wellington, Wellington, New Zealand, [2]Victoria University of Wellington, Wellington, New Zealand, [3]Victoria University of Wellington, Wellington, New Zealand

Session 4A: Electrocatalysis, Auditorium, February 11, 2025, 10:40 - 12:45

Bubble nucleation is a problem that affects the performance of electrocatalytic reactions in oxygen evolution reactions (OER) because it blocks the active sites. When the bubble is extremely small, on the order of nanometers, the problem becomes more challenging to localise the electrochemical measurements and correlate those with high-resolution imaging. This limitation presents a significant challenge in exploring the stochasticity and spatial heterogeneity inherent in nanoelectrochemical interfaces. Understanding the activities across different surface facets is crucial for designing high-performance electrocatalysts for oxygen evolution reactions.

In this study, we reproducibly generated and characterised single oxygen nanobubbles on nickel surfaces using the Scanning Electrochemical Cell Microscopy (SECCM) method. In scan hopping mode, the SECCM probe conducts local cyclic voltammetry at a predefined grid location to get the nanoelectrochemical activities, which then can be compared with the characterisation images from Scanning Electron Microscope-Electron Backscatter Diffraction. We used 1M KOH solution and the opening tip radius of ~250 nm nanopipette to detect high mass-transport rates and provide a mapping of the electrocatalytic activity associated with OER on various nickel surface facets.

Our findings show that oxygen nanobubbles form at different dissolved oxygen concentrations on different crystal facets and grain boundaries of nickel. This offers new insights into the structure-activity relationships that govern OER performance. Our results significantly affect the development of efficient nickel electrocatalysts with reduced bubble formation.

Electrochemistry of V5+/4+ reaction on catalytic heteroatom-doped carbon electrode derived from ionic liquids

Mr Pitambar Poudel[1], Dr Chang Wu[1], Dr Aaron T. Marshall[1]
[1]Department of Chemical and Process Engineering, The MacDiarmid Institute for Advanced Materials and Nanotechnology,University of Canterbury, Christchurch, New Zealand

Session 4A: Electrocatalysis, Auditorium, February 11, 2025, 10:40 - 12:45

Carbon-based materials for various electrochemical applications can be produced through the pyrolysis of ionic liquids (ILs). However, in many cases, at the high-temperature conditions used for the pyrolysis, IL like tris(dibutylamino)cyclopropenium bis(2-ethylhexyl)phosphate ([TDBaCp][BEHB]), can have significant volatility, resulting in very low yields (< 0.5%) of the final carbon material. Mixing carbon materials (e.g., carbon black, graphene, or carbon nanotubes) into the IL prior to carbonisation, can dramatically increase the yield of IL-derived carbon produced by pyrolysis. In this work, IL-derived carbons were prepared and characterised using X-ray photoelectron spectroscopy, N2 adsorption/desorption isotherms, Raman spectroscopy, electrochemical impedance spectroscopy (EIS) and cyclic voltammetry. The electrochemical behaviour of the V5+/4+ redox reaction was examined at a carbon-modified electrode using three-electrode rotating disc electrode (RDE) voltammetry. The results demonstrated improved electrochemical activity and kinetics for the IL-derived carbon material in V5+/4+ redox couples compared to both pre-made carbon-fabricated glassy carbon RDE and the glassy carbon RDE itself. The activity, assessed by peak potential separation (ΔEp), was further confirmed by EIS. A correlation was observed between the presence of heteroatoms such as N, S, and P in the IL-derived carbon, which increased structural disorder (as indicated by Raman spectroscopy) and enhanced activities. Additionally, the presence of oxygen-functionalized groups in the derived carbon was found to improve surface wettability. These findings suggest that IL precursors could be used to produce functionalized carbon electrodes suitable for vanadium redox flow battery applications.

Electroreduction of NO3- to N2 on Pt(111) and Pd(111) Surfaces

Samantha (Sam) McIntyre[1,2], Dr Caitlin Casey-Stevens[1,2], Dr James Thomas Gilmour[1,2], Dr Charlie Ruffman[1,2], Dr Anna Garden[1,2]
[1]University Of Otago - Department of Chemistry, Dunedin, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, New Zealand

Session 4A: Electrocatalysis, Auditorium, February 11, 2025, 10:40 - 12:45

In recent years, reactive nitrogen species have become prevalent pollutants in the biosphere with nitrate (NO_3-) in particular, causing substantial contamination of terrestrial waterways and ground water.[1] Therefore, research has focused on designing catalysts which are able to reduce nitrate levels by converting these threatening pollutants into benign products such as N_2.[1,2] One method which has shown promise is the electrocatalytic reduction of NO_3- to N_2 under acidic conditions using a Pd(111) surface.[2] Curiously, while Pd and Pt exhibit similar catalytic behaviour for many reactions, the Pt(111) surface does not behave similarly with respect to the selective nitrate reduction, producing predominantly NH_4+ and N_2O, with little to no N_2 produced.[3]

In this work, density functional theory is used to study the formation of N_2 from NO on both Pt(111) and Pd(111). It is found that both metals exhibit a similar mechanism and energy profile for N_2 formation. However, they exhibit key differences in hydrogen adsorption behaviour. Therefore, hydrogen coverage as a function of electrode potential is explored in more detail, using statistical modelling, to see whether surface hydrogen atoms may inhibit the formation of N_2 on Pt(111) and explain the differences in observed selectivity.

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From Microfluidics to Engineering Thermodynamics - An Overview of the Energy Technology Lab at Otago

Dr Sam Lowrey[1]
[1]University of Otago, Dunedin, New Zealand, [2]Dodd-Walls Centre for Photonic and Quantum Technologies, New Zealand

Session 4B: Microfluidics, Dobson 1, February 11, 2025, 10:40 - 12:45

Nature has evolved impressive water management solutions. The most cited and well-known example is the super water-repellent lotus leaf, which has a surface consisting of random microscale bumps with superimposed nanoscale hairs covered in wax [1]. In addition, the Cicada has evolved wings that are not only superhydrophobic, but also promote a gradient in surface tension, allowing for rapid water removal [2].

Adopting these water management solutions found in nature could lead to vastly improved energy systems in terms of energy efficiency. For example, such surfaces (1) promote dropwise condensation over film-wise, improving water droplet removal, which is beneficial for heat exchangers, and (2) promote delay (or elimination) of ice-/frost-formation under extreme weather conditions, which may be beneficial for wind turbine blades.

This presentation will summarise research conducted at Otago on coating-less, topographical wetting gradients. We have developed design tools, fabrication methods, and testing procedures for these surfaces, which can be produced on metal using a simple, industrial process [3],[4]. These surfaces have been assessed for their durability and stability under various conditions, and the results will be presented. We will also present our more recent work into investigating: scale-up of these surfaces, extending these gradients to curved surfaces, confined droplet behaviour, and other conditions including forced vibration, condensation and coalescence, all with the aim of moving this surface technology closer to real-world energy applications. Our investigations into heat exchanger and heat pump technology will also be briefly discussed, specifically in its relation to our microfluidics research.

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Taking spin coating to another dimension

Mr Finn McIntyre, Matthew Bayley[3], Associate Professor Shayne Gooch[3], Professor Mathieu Sellier[3]
[1]Electrical and Computer Engineering, University of Canterbury, Christchurch, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand, [3]Mechanical Engineering, University Of Canterbury, Christchurch, New Zealand

Session 4B: Microfluidics, Dobson 1, February 11, 2025, 10:40 - 12:45

Due its simplicity, spin coating remains a preferred method for producing thin film layers. The technique is used in the manufacture of a large and diverse number of consumer products ranging from smartphones to sunglasses and solar panels. Spin coating also continues to play a crucial role in photolithography, the key process driving miniaturization of integrated circuits, despite major technological changes, such as the recent move to extreme UV lithography. Traditionally used to apply uniform films to flat, rigid substrates, rising interest in electronics on organic, curved shapes that interface with our bodies [1], has created a need to explore spin coating's suitability for non-planar substrates [2,3]. To aid in this, we have recently introduced a novel multi-axis manipulator and associated characterisation equipment, creating a platform technology to controllably deposit thin films onto curved surfaces [4,5]. Supported by modelling and simulation [6-8], this has allowed us to evolve the traditional spin coating technique into a tool to form curved polymer coatings with improved thickness control. In this work we will present our latest coating results, as well as the use of this coating technique to form photoresist films on spherical and cylindrical substrates. Furthermore, we will show how these films can be used in conjunction with UV photolithography and flexible masks to define arbitrary patterns on these substrates.

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Investigating Dynamics of Janus Particles using Microfluidic Devices

Mr Stephen Chung[1,2], Prof. Volker Nock[1,3], Prof. Geoff R. Willmott[1,2,4]
[1]Department of Physics, The University Of Auckland, Auckland, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, [3]Department of Electrical & Computer Engineering, University of Canterbury, Christchurch, New Zealand, [4]School of Chemical Sciences, The University of Auckland, Auckland, New Zealand

Session 4B: Microfluidics, Dobson 1, February 11, 2025, 10:40 - 12:45

Janus particles are asymmetric colloids that show great promise for technological advancements which use nano- and micro- scale self-assembly and reconfiguration. The anisotropic nature of these particles introduces directionality in particle-particle interactions, and for amphiphilic particles these interactions may be dominated by hydrophobic attraction [1]. However, further study is needed to better understand the dynamics of these interactions [2]. There is a particular opportunity to control and observe these dynamics by suspending Janus particles in continuous flows within microfluidic channels.

In the present work, we are developing sheath-flow microfluidic channels to study the dynamics of Janus particles. We use photolithography and two-photon polymerisation to fabricate various microfluidic devices to characterise the particle dynamics. A custom-built optical microscope has been set up to observe the microfluidic channels in two directions, and an image analysis program developed using Python is used to gather information about the dynamics of Janus particles as they travel through the channels. We characterise particle-particle interactions and inertial effects by measuring particle position and orientation as a function of their position and the surrounding flow profile. Our latest results and analysis of these experiments will be presented.

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Rapid In-Situ Bacterial Detection Using Nanostructured Surfaces and Microfluidics

Dr Amal Senevirathne[1], Prof Prasad Yarlagadda[1]
[1]Queensland University of Technology, Brisbane, Australia

Session 4B: Microfluidics, Dobson 1, February 11, 2025, 10:40 - 12:45

Bacterial infections are a leading cause of mortality worldwide, contributing to millions of deaths annually and imposing significant economic burdens across multiple sectors, including healthcare and agriculture (Ikuta et al., 2022; Brooks & Flint, 2008; Cobo-Díaz et al., 2021). The global economy stands to lose a projected 3.8% of its annual GDP by 2050 due to bacterial contamination (Cobo-Díaz et al., 2021), underlining the urgent need for effective and timely detection methods. Current bacterial detection techniques, such as culture-based methods, although reliable, are time-consuming and can take up to 72 hours to yield results (Huber et al., 2022). While rapid detection techniques like antigen tests exist (Farhoudi et al., 2019; Huber et al., 2022), they often lack sensitivity and require sophisticated laboratory infrastructure, making them unsuitable for in-situ or large-scale applications.

This research seeks to address these challenges by developing an innovative bacterial detection method that leverages the unique properties of nanostructured surfaces combined with microfluidic techniques. Nanostructured surfaces have been shown to enhance bacterial adhesion under fluid shear conditions (Senevirathne et al., 2022, 2023; S.W.M.A.I. Senevirathne, 2022), a property that can be exploited to trap and concentrate bacterial cells from samples with low bacterial loads; conditions that are more representative of real-world clinical and industrial scenarios. By manipulating the sample volume and exposure time using microfluidic methods, it’s aimed to create a rapid, highly sensitive detection system.

The proposed research is to be undertaken with mixed bacterial populations and clinically relevant bacterial loads, offering a realistic simulation of infection and contamination scenarios. The proposed method not only reduces detection time but also improves sensitivity, making it a viable alternative to existing technologies. The development of this technique holds significant commercialization potential, with applications in medical diagnostics and industrial contamination detection, offering a faster, more efficient, and cost-effective solution to one of the most pressing global health challenges.

Using Lab on a Chip to investigate the invasive biology of pathogenic fungi and oomycetes

Dr Ayelen Tayagui[1,2,3], Dr Yiling Sun[1,3], Dr Sarah Sale[1,2,3], Ms Debolina Sarkar[2], Professor Volker Nock[1,3], Associate Professor Ashley Garrill[1,2]
[1]Biomolecular Interaction Centre, Electrical and Computer Engineering, University of Canterbury, Christchurch, New Zealand, [2]School of Biological Sciences, University of Canterbury, Christchurch, New Zealand, [3]The MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand

Session 4B: Microfluidics, Dobson 1, February 11, 2025, 10:40 - 12:45

Oomycetes and fungi are filamentous microorganisms that are among the most destructive plant and animal pathogens known. The diseases they cause are responsible for significant loss of biodiversity and current estimates put crop, horticultural, forestry and aquaculture losses in the billions of US$ annually1. They spread via micrometre-sized spores, which locate their hosts and germinate forming invasive cells called hyphae, that penetrate and break down host tissue2. To better understand the mechanisms, they use to locate and invade their hosts, we have designed and demonstrated a number of Lab-on-a-Chip platforms and associated characterisation techniques3-7. In this paper I will give an overview of these systems, which we are developing to study the invasion process at various points along the pathogen life-cycle, including spore survival in the environment, propulsion to and external interaction with host plant surfaces, generation of mechanical force by germ tubes and hyphae to invade the host cells, as well as biomaterial and RNAi-based control methods to reduce the impact of these pathogens. In particular, I will describe our recent efforts to miniaturize force sensing pillars using 2-photon polymerization 3D printing, as well as to develop novel spore compartmentalization devices to study the biophysical and biochemical changes happening during turgor regulation in oomycetes.

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CRISPR-Aptamer Integration: A Novel Approach for Robust and Cost-Effective Small Molecule Drug Testing

Dr Anindita Sen[1]
[1]Institute of Environmental Science and Research, Wellington, New Zealand

Session 4B: Microfluidics, Dobson 1, February 11, 2025, 10:40 - 12:45

Aptamers, synthetic DNA or RNA molecules, are designed to bind small molecules with high specificity and affinity making them as attractive tools in drug testing. However, practical implementation presents significant challenges. Real-world samples often introduce matrix effects that interfere with specificity and sensitivity, and translating aptamer performance from laboratory conditions to applied settings frequently reveals limitations in stability and robustness. Developing aptasensors for small molecules remains particularly challenging due to the small size of the targets, which often results in negligible conformational changes. This makes signal transduction difficult, especially in sensors requiring aptamer immobilization on surfaces such as electrodes.

A key case-study involves the use of gold nanoparticle-based aptasensors for methamphetamine detection in saliva. This case study underscores the complexities of deploying aptamers in downstream sensing platforms and their subsequent application in complex biological samples. These limitations motivated the development of alternative strategies, emphasizing the need for a robust, generalizable solution that performs reliably across diverse conditions.

To address these challenges, we propose a novel aptasensing technology combined with DNA-based fluorescent reporting using CRISPR/Cas systems to detect illicit substances. This approach involves using aptamers for initial target recognition, which subsequently activates the CRISPR-Cas complex to generate a fluorescent signal. The envisioned platform is a cost-effective, paper-based matrix, providing a disposable solution to expand the scope of diagnostics for illicit substance detection.

Development of an Automated Microfluidic Ion Pipette Aspiration System for Analysing Viscoelastic Micro-particles

Mr Chi Minh Truong[1,2,6], Doctor Ayelen Tayagui[1,3,4], Professor Volker Nock[1,3], Associate Professor Ashley Garrill[4], Professor Frederique Vanholsbeeck[2,6], Professor Geoff Willmott[1,2,5]
[1]The MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand, [2]Department of Physics, The University of Auckland, Auckland, New Zealand, [3]Department of Electrical and Computer Engineering, University of Canterbury, Christchurch, New Zealand, [4]School of Biological Sciences, University of Canterbury, Christchurch, New Zealand, [5]School of Chemical Sciences, The University of Auckland, Auckland, New Zealand, [6]The Dodd-Walls Centre for Photonic and Quantum Technologies, Otago, New Zealand

Session 4B: Microfluidics, Dobson 1, February 11, 2025, 10:40 - 12:45

The mechanical properties of tissues and cells in a living body can provide important insights into biological functions [1], health conditions [2], and disease development [3] of the entire system. Ion pipette aspiration (IPA) [4] is a measurement method for these properties in cells, micro-organisms [5], and a growing number of nanoengineered colloidal technologies. IPA integrates conventional micropipette aspiration (MA) with resistive pulse sensing (RPS) to measure sample deformation and resistivity changes of the sample under negative pressure. This presentation will describe efforts to develop a compact automated microfluidic IPA system with improved throughput and measurement accuracy. This system consists of three main components, the microfluidic MA structure, the RPS system, and the microscope camera system. The microfluidic MA part requires a constriction such as a borosilicate micropipette to be embedded inside of a chip, with a microscope camera typically used to optically measure the sample deformation during MA. The RPS part uses electrodes embedded near the constriction to precisely monitor current changes. A complete IPA system combines these components together with a control system and development of models linking mechanical properties to experimental data. This type of device is well suited for profiling and comparing the mechanical properties of biological particles and has the potential to be used for analysis of nanoscale particles.

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Silicon carbide as a platform for mid-IR metasurfaces

Dr Stefan Maier[1]
[1]Monash University, Melbourne, Australia

Session 4C: Photonics, Dobson 2, February 11, 2025, 10:40 - 12:45

Surface-phonon polaritons, hybrid light/matter modes based on the coupling between the electromagnetic field and transverse optical phonons in the restrahlen band of polar dielectrics, are a promising route towards deep sub-wavelength mid-IR photonics. We examine the use of silicon carbide as a platform for surface phonon-polariton metasurfaces. Thin membranes of this material allow for the generation of even and odd surface phonon-polariton coupled modes, the dispersion of which we investigate using near-field optical microscopy. Structuring of the sicilon carbide surface then enables the creation of functional mid-IR photonics structures, which we demonstrate for the cases of vortex modes and quasi bound-state-in-the-continuum resonances. We further present geometries based on out-of-plane symmetry breaking as a means for tailored surface enhanced infrared absorption (SEIRA) sensing with a metallic metasurface.

Giant magnitude of ultraviolet magnetic circular dichroism in thin film Co2MnGa1-xGe1-x Heusler alloys

Dr Simon Granville[1,2], Yao Zhang[1], Yuefeng Yin[3], Hua-Shu Hsu[4]
[1]Victoria University of Wellington, Lower Hutt, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand, [3]Monash University, Clayton, Australia, [4]National Pingtung University, Pingtung, Taiwan

Session 4C: Photonics, Dobson 2, February 11, 2025, 10:40 - 12:45

Ferromagnetic Weyl semi-metal Heusler alloy Co_2MnGa has been shown to have very large values for a range of magnetoelectronic properties such as large anomalous Hall [1,2], anomalous Nernst [3,4], and spin Hall [5] coefficients, related to the large Berry curvature in this material's electronic structure. The strongly spin-polarised band structure might be expected to show up in spin-selective optically-excited transitions between the states, which may have applications in magneto-optics, however optical and magneto-optical studies of Co_2MnGa are much less common [6,7].

In this presentation we will show a giant difference in the absorption of right- and left-circularly polarised UV light in Co_2MnGa1-xGe1-x thin films, reversible with a magnetic field. This magnetic circular dichroism (MCD) reaches over 25 mdeg/nm, almost as large as the strongest UV MCD in rare-earth-containing ferromagnets such as CoTb or GdFeCo. The MCD has the same magnetic field dependence as the anomalous Hall effect, evidence it is linked to the electronic band structure. From calculations of the spin-polarised density of states, we link the MCD to optical transitions between hybridised Co-Mn 3d minority states. Substituting Ge for Ga broadens the large MCD response to cover a wide range of UV energies, 3.5 – 4.5 eV. Our results demonstrate these materials are a promising way to achieve large and broad MCD for applications with immunity to temperature variation.

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Ultrafast UV Luminescence in ZnO Films Fabricated by MF+ECWR Magnetron Sputtering

Dr Jiri Olejnicek[1], Dr. Marilou Cadatal-Raduban[2,3], Aneta Pisarikova[1], Dr. Michal Kohout[1], Dr. Lenka Volfova[1], prof. Rainer Hippler[1], prof. Nobuhiko Sarukura[3], prof. Shingo Ono[4], prof. Kohei Yamanoi[3], Dr. Zdenek Hubicka[1]
[1]Institute of Physics of Czech Academy of Sciences, Prague, Czech Republic, [2]Unitec Institute of Technology, Auckland, New Zealand, [3]Osaka University, Institute of Laser Engineering, Osaka, Japan, [4]Nagoya Institute of Technology, Nagoya, Japan

Session 4C: Photonics, Dobson 2, February 11, 2025, 10:40 - 12:45

Ultrafast luminescence is a critical requirement in fast-timing applications, where time resolution below 100 ps is necessary. This study focuses on the development of undoped ZnO thin films, several microns thick, deposited on cost-effective soda lime glass substrates using three different physical vapor deposition (PVD) techniques. The methods employed include: (i) pulsed DC hollow cathode discharge utilizing a metallic zinc target, (ii) DC magnetron sputtering from a ZnO ceramic target, and (iii) medium frequency (MF) magnetron sputtering combined with electron-cyclotron wave resonance (ECWR) plasma. The techniques (i) and (iii) involved reactive sputtering in an Ar/O_2 atmosphere, while the second method utilized pure Ar gas. X-ray diffraction confirmed that all deposited ZnO layers exhibited a wurtzite structure with a predominant (002) orientation. Notably, the ZnO layers fabricated using the MF+ECWR method demonstrated an exceptionally high UV luminescence intensity with a peak wavelength of 382 nm, surpassing the other techniques by a factor of ten. Furthermore, these layers exhibited ultrafast decay times in the range of 9 to 25 ps, making them ideal for high-precision optical applications. The study also examined the effects of substrate temperature during deposition and post-deposition annealing, revealing that these factors significantly influence the crystallographic and photoluminescent properties of the ZnO films. The results of this research underscore the potential of MF+ECWR sputtering technology for producing high-performance ZnO films with superior UV luminescence, paving the way for advancements in optical sensing and other related fields.

Enhancing upconversion efficiency in lanthanide systems with tunable silver plasmonic nanoparticles

Mrs Romina Marie Mathew[1]
[1]Aut, Auckland, New Zealand

Session 4C: Photonics, Dobson 2, February 11, 2025, 10:40 - 12:45

Photon upconversion, the process of converting lower-energy photons into higher-energy photons, holds significant potential for applications in bioimaging, light harvesting, photocatalytic cells, and optical probes[1], [2], [3]. Upconversion nanoparticles (UCNPs), such as NaYF4 doped with lanthanide ions (e.g., Yb^{3+} and Er^{3+}), are particularly promising due to their ability to emit higher-energy photons (blue or green) when excited by lower-energy photons[4], [5]. However, their current upconversion efficiencies are often limited for practical use, limiting their real-world applications.

It is possible to modulate transition rates in a chromophore by coupling to resonant localised surface plasmons in nearby metal particle[6]. In this project, our aim is to explore the ability of silver nanoparticles (NPs) to enhance upconversion rates in co-located lanthanide-containing UCNPs. To achieve this, we are synthesising NPs with frequencies tuned to match those of the Ln3+ ions in our UCNPs. These are then fabricating into monolayer films onto which we are coating a layer of UCNPs.

Here, we present our synthesis and thin-film fabrication experiments, together with the results from time-resolved luminescence studies on silver and lanthanide NP systems. We will demonstrate the changes in excited state dynamics that are observed when lanthanide systems are coupled to resonant surface plasmons and describe how these could be used to enhance upconversion.

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Luminescent Materials with Memory are Optically Memristive Systems

Dr Joseph Schuyt[1], Mr Andrew Sutcliffe[1], Prof Grant Williams[1], Dr Shen Chong[1]
[1]Victoria University of Wellington, Wellington, New Zealand

Session 4C: Photonics, Dobson 2, February 11, 2025, 10:40 - 12:45

Photostimulated and persistent luminescence phenomena arise in optical materials that can absorb and store energy in meta-stable charge traps. The stored energy can be released upon some suitable optical or thermal stimulation, whereupon a luminescent output is observed. As the stored energy may contain information, these materials are considered luminescent materials with memory. To date, photostimulated and persistent luminescence phosphors have found numerous applications primarily associated with optical sensing, spanning physical, chemical, and biological spaces [1][2]. However, recent research has focused on potential applications in future computing networks, as data storage media [3] and as neuromorphic computing elements [4].

In this work, we demonstrate that some luminescent materials with memory are prototypical memristive systems, using the original memristive formalism [5]. The inputs are optical stimulations that fill or empty trap states, and the outputs are luminescence signals. They therefore function as all-optical luminescent memristive systems, i.e., memlumors [6]. Using dynamic charge transport models, we demonstrate that these phosphors are theoretically memristive and model the memristive properties. Then, using a model photostimulable phosphor and a model persistent phosphor we experimentally validate our stimulations, and conclusive demonstrate that memristive and pseudo-memristive behaviours emerge in luminescent materials with memory. Our demonstration encourages further research into these materials for future computing applications reliant on non-linear memristive effects.

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Multi-wavelength lasing via self-frequency conversion in GaNAs-based nanowires

Dr Mattias Jansson[1], Dr Valentyna Nosenko[1], Mr Yuto Torigoe[2], Mr Kaito Nakama[3], Mr Mitsuki Yukimune[2], Mr Akio Higo[4], Prof. Fumitaro Ishikawa[3], Prof Wei Min Chen[1], Professor Irina Buyanova[1]
[1]Linkoping University, Linkoping, Sweden, [2]Ehime University, Matsuyama, Japan, [3]Hokkaido University, Sapporo, Japan, [4]University of Tokyo, Tokyo, Japan

Session 4C: Photonics, Dobson 2, February 11, 2025, 10:40 - 12:45

Nanowire (NW) lasers made of semiconductors offer numerous advantages for future integrated photonic devices. Dilute nitride III-N-V alloys represent an attractive material system for these applications as the giant bandgap bowing in these materials [1] offers increased flexibility in tuning lasing wavelength [2, 3]. In this work, we explore nonlinear optical phenomena in the dilute nitride NWs aiming at achieving multi-wavelength lasing.

The investigated GaAs/GaNAs/GaAs core/shell/cap NWs were fabricated using selective area growth during molecular beam epitaxy on patterned Si substrates. We found [4] that the fundamental laser light in these structures experiences self-frequency conversion through second harmonic generation and sum-frequency generation leading to coherent light emission within the technologically challenging cyan-green spectral range. The self-conversion efficiency varies between different fundamental lasing modes: it is the lowest for the HE11b mode but is enhanced by more than two orders of magnitude for the HE21b mode. Based on the performed finite-difference time-domain simulations, we attribute these differences to the combined effects of different electric field distributions of the fundamental lasing modes inside the NWs, their different light extraction efficiencies, as well as an improved non-linear response of the GaNAs alloys as compared with parental GaAs. Moreover, the upconverted emission is observed at temperatures up to 200 K, which is significantly higher than the previously reported temperature of 10 K for self-frequency conversion in InGaAs NWs [5]. Our work, therefore, advances the performance of GaNAs-based NW lasers paving the way for the development of multi-wavelength coherent light generation and room temperature applications of GaNAs-based NW lasers.

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Plasmon-coupled optical properties of molecular chromophores with resonance-tuned silver nanoparticles

Miss Róisín Mooney[1], Taniela Lolohea[1], A/Prof Marcus Jones[1]
[1]School of Science, Auckland University of Technology, New Zealand

Session 4C: Photonics, Dobson 2, February 11, 2025, 10:40 - 12:45

Plasmonic silver nanoparticles offer a highly tunable platform for modulating radiative and non-radiative processes in nearby chromophores. To probe these interactions, it is essential to maintain narrowly distributed nanoparticle morphologies and well-controlled silver-tochromophore distances. We have developed optimised protocols for the synthesis and purification of silver nanorods and nanoplates with narrow size and shape distributions. Their absorbance and scattering resonances can be tuned across the visible and through the NIR spectral window, enabling them to be adapted to a wide range of chromophores.

We have also developed a robust method for fabricating monolayer silver nanoparticle films that can be overlayed with molecular chromophores. This fabrication method has enabled a high degree of control over the particle density and interparticle proximity, thereby modulating plasmon-chromophore coupling. We will present the results of these studies and illustrate the influence of a resonance-tuned plasmonic sub-layer on the steady-state and time-resolved fluorescence of rubrene thin films. Ultimately, these systems could be used to increase efficiency in light-harvesting or photo-emission applications.

Towards High-Throughput Rational Design of Organic Solar Cells and Semiconductor Materials using Machine Learning and Computational Chemistry

Dr Geoffrey Robert Weal[1,2,4], Dr. Chayanit Wechwithayakhlung[1,4], Dr. Joshua J Sutton[2,3], Prof. Justin M Hodgkiss[2,3,4], Dr. Paul A Hume[2,3,4], Assoc. Prof. Daniel M Packwood[1,4]
[1]Institute for Integrated Cell-Material Sciences (iCeMS), Kyoto University, Kyoto, Japan, [2]School of Chemical and Physical Sciences, Victoria University of Wellington, Wellington, New Zealand, [3]MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand, [4]Center for Integrated Data-Material Sciences (iDM), Wellington, New Zealand

Session 4D: Computational, Dobson 3, February 11, 2025, 10:40 - 12:45

Organic photovoltaics (OPVs) offer exciting possibilities for lightweight, flexible, and printable solar panels that can not be achieved with current silicon-based technologies.(1,2) Accurate property prediction is paramount to high-throughput computational screening of OPV materials with superior solar power efficiencies. This is challenging because many key processes that affect solar efficiencies depend on both intra- and inter-molecular properties, such as exciton (electron-hole pair) diffusion about organic devices.(3,4)

The goal of this project is to drastically reduce the time and computational resources required to make accurate predictions of exciton diffusion and other properties in organic semiconductors.

In this talk, we will:

1. Discuss a protocol we have devised to investigate the intermolecular properties of OPV materials,(5) and how we have scaled this up for high-throughput calculations of 2300 crystal structures, consisting of ~4000 molecules.
2. Show that our protocol accurately predicts the ordering of exciton diffusion rates compared to experiment for several existing high-performance OPV devices using kinetic Monte Carlo and a sum-over-rates equation,(5) and
3. Explain how we are using machine learning (such as graph neural networks) and other techniques to speed up exciton coupling and other solar/electronic property predictions.(5)

Our results reveal a viable path toward high-throughput virtual screening of organic semiconductors. In the future, we hope this protocol can be used by both computational and non-computational researchers as another tool in the toolbox to investigate organic semiconductors.

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Computational design of catalytic nanomaterials for oxidative abatement of air pollutants at very low temperatures

Professor Konstantin Neyman[1], Pablo Castro-Latorre, Jon Quinlivan, Dr. Albert Bruix
[1]Icrea & Universitat De Barcelona, Barcelona, Spain

Session 4D: Computational, Dobson 3, February 11, 2025, 10:40 - 12:45

Reducing the operating temperature of oxidation catalysts is important for designing energy-efficient processes, extending catalyst lifetime, and abating pollutants, especially in cold conditions. CO oxidation activity at sub-ambient temperatures is reported for Pt/CeO2 catalysts containing Pt cations [1]. Our density functional calculations revealed a surprisingly high thermodynamic stability of small supported on CeO2 oxidized PtOx clusters at very low oxygen pressure and room temperature [2]. The PtOx clusters are found to be notably more stable than the metallic platinum clusters with the same number of Pt atoms and comparable in the stability with the single-atom Ptn+ species.

This work explains, how the ceria-supported PtOx clusters trigger CO oxidation well below room temperature [3] and what makes them so efficient in the oxidation process [4]. Thus advanced atomic-level understanding of the catalytic oxidative function of the PtOx/CeO2 nanomaterials paves the way to design catalysts for oxidative abatement of air pollutants at very low temperatures, even without using precious metals and other critical elements.

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A Divide and Conquer Approach to Nanoparticle Global Optimisation

Mr Nicholas Smith[1,2], Assoc. Prof. Anna Garden[1,2]
[1]University Of Otago, Dunedin, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand

Session 4D: Computational, Dobson 3, February 11, 2025, 10:40 - 12:45

Metallic nanoparticles exhibit unique electrical, mechanical and optical properties that are distinct from bulk metal, lending them to exciting applications as catalysts such as for the CO_2 reduction reaction[1] or hydrogen evolution reaction.[2] However, the structures adopted by nanoparticles are a key determinant of their properties, including their catalytic activity, and the computational prediction of these structures remains a fundamental issue in nanoparticle chemistry.[3] This task, performed by global optimisation algorithms, aims to locate the lowest energy structure (the global minimum) on a vast potential energy surface (PES), with some driver pushing the search towards low energy regions. However, high energy barriers often exist between low energy regions, separating the PES into multiple funnels which hampers the ability of the algorithm to explore all but the broadest of these funnels. This multi-funnel effect is especially problematic when the global minimum is located within a narrow funnel.[3,4]

A divide-and-conquer approach has the potential to improve the efficiency of global optimization algorithms in solving multi-funnel systems. This approach involves identifying the distinct funnels and conquering them separately. The question then becomes how these funnels can be identified, and the PES divided. Examples exist in the literature of this paradigm being applied successfully to specific nanoparticles, however, these examples apply a priori knowledge of the system in the division scheme.[5,6] This presentation will detail how we applied machine learning to achieve this separation, without a priori knowledge, and the impact this scheme had on the speed of locating difficult to find structures.

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Elucidating the Electrolytes Involved in the Solvation of Vanadium Ions in the Catalytic Reactions within Redox Flow Batteries

Mr Christopher Mills[1], Associate Professor Anna Garden[1]
[1]University Of Otago, Dunedin, New Zealand

Session 4D: Computational, Dobson 3, February 11, 2025, 10:40 - 12:45

This project focuses on developing vanadium redox flow batteries (VRFBs) for energy storage from renewable sources like wind and solar. VRFBs utilise the redox states of soluble vanadium species, offering high energy densities, long lifespans, and near-complete discharge.[1] However, their slow reaction rates at catalytic electrode surfaces hinder commercial viability.[1,2] In VRFBs, redox reactions occur at the positive ($VO^{2}+/VO_{2}+$) and negative ($V^{2}+/V^{3}+$) electrodes:[2]

Positive electrode: $VO_{2}+ + 2H+ + e- \rightarrow VO^{2}+ + H2O$ (1)
Negative electrode: $V_{2}+ \rightarrow V^{3}+ + e-$ (2)

One significant challenge in vanadium redox flow batteries (VRFBs) is understanding the underlying mechanisms of their reactions.[2] Current understanding suggests that reactions at the positive and negative electrodes follow outer- and inner-sphere mechanisms, respectively, likely due to differences in their solvated structures.[2] This project investigates the solvated structures of vanadium ions with common electrolytes using computational techniques like ab initio and classical molecular dynamics, and density functional theory. This investigation is crucial for gaining a deeper understanding of solvation spheres, which has the potential to influence reaction kinetics. Additionally, we will examine both proposed and novel reaction mechanisms using pristine and functionalised carbon-felt models and explore surface modification techniques to enhance catalytic activity.

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Melting of noble gas systems under extreme conditions

Miss Diana Yu[1]
[1]Miss. Diana Yu, Auckland, New Zealand

Session 4D: Computational, Dobson 3, February 11, 2025, 10:40 - 12:45

The discovery of strong magnetic fields on magnetic white dwarf stars (B ≈10^2 to 10^5 T), and neutron stars (B ≈ 10^7 to 10^9 T) has led to great interest in the study of matter under such conditions. We use Monte Carlo simulations to study the melting of noble gas systems, mainly helium, neon and argon under strong magnetic fields and high pressure [1].

Due to a bonding mechanism found under magnetic field called perpendicular paramagnetic bonding [2], the interaction energy between atoms depends on the angle between their bond and the magnetic field, with the bonding being stronger and the equilibrium distance being shorter when the bond and the field direction are perpendicular to each other. The traditional cubic shaped periodic boundary introduces bias under such circumstances, when the atoms attempt to rearrange into layers perpendicular to the magnetic field and form gaps near the edge of the box. Therefore, we introduce a right rhombic prism-shaped box, where the ratio between the lengths of its edges can change. We compare the melting curve obtained using the cubic box and the rhombic box.

The rhombic box can accommodate both fcc and hcp structures if a correct number of layers is chosen. In order to find possible structural transitions, we have adopted an algorithm based on common neighbour analysis and machine learning [3][4][5] to determine the structural motifs of a large number of configurations recorded during the simulations.

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Probing Reaction Mechanisms on a Membrane Using Metadynamics Simulations

Dr Brandon Meza González[1,2], Professor Daniel Packwood[1]
[1]Kyoto University iCeMS, Kyoto, Japan, [2]National Autonomous University of Mexico, Mexico City, Mexico

Session 4D: Computational, Dobson 3, February 11, 2025, 10:40 - 12:45

Paraoxon is an emerging organophosphate compound widely used both as a pesticide and a drug [1]. Given the high toxicity and tendency to accumulate in organisms associated with organophosphate compounds, numerous methods have been developed to facilitate their degradation and removal.

The existing approaches available for the degradation of organophosphate compounds include homogeneous and heterogeneous hydrolysis, photolysis, photochemical degradation, and biodegradation [2].

In this work, we employ the Well-Tempered Metadynamics (MTD) formalism to reconstruct the Free Energy Surface associated with paraoxon hydrolisis on a membrane model.

The Metadynamics approach can yield a fine image of the minimum energy pathway connecting two meta-stable states, providing detailed reaction pathways and their associated energetics. Thus, it minimizes scientific bias by automatically building the reaction coordinate. MTD accelerates the sampling of events and inherently explores the low free energy regions of a system. In contrast, quantum static calculations explore individual routes, which can lead to a bias in initial structures and preferred pathways [3].

Specifically, the membrane model consists of bipyridine motifs grafted to a polypropylene backbone. On top of these motifs copper atoms form complexes that catalyze the hydrolisis. The model predicts that the membrane-supported catalyst improves the catalytic hydrolysis of paraoxon. The study proposes that future membrane-supported catalysts should maximize substrate-polymer interactions to reduce energy barriers and improve catalytic efficiency.

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Accurate representation of hydrogen in metals by machine-learning enhanced modelling of nuclear quantum effects

Dr Kai Sellschopp[1], Prof Thomas Klassen[1,2], Dr Paul Jerabek[1], Dr Claudio Pistidda[1]
[1]Helmholtz-Zentrum hereon, Geesthacht, Germany, [2]Helmut Schmidt University, Hamburg, Germany

Session 4D: Computational, Dobson 3, February 11, 2025, 10:40 - 12:45

In a sustainable economy built on renewable energy, hydrogen plays a key role for storing energy and replacing fossil fuels. An efficient way to store hydrogen is to keep it in the solid state by binding it chemically in a metal hydride, which is particularly useful for seasonal energy storage or for applications where safety is a concern. Hydrogen is known to show nuclear quantum effects (NQE), such as high delocalisation and tunneling through energy barriers, even at elevated temperatures. Additionally, the bonding situation in many metal hydrides gives rise to an anharmonic potential energy surface (PES) in the vicinity of typical hydrogen positions. Technically, an accurate representation of Hydrogen in metals therefore needs to take anharmonic NQE into account, but these have been mostly neglected in computational studies so far due to the high cost of the associated path-integral molecular dynamics (PIMD) calculations. In this work, a machine-learned potential (MLP) is trained to approximate the PES of the Mg-H system, a well-known hydrogen storage material, to speed up the simulations and bring down the cost of NQE calculations. Combining "on-the-fly" training with PIMD sampling results in highly accurate MLPs and an efficient workflow that is transferable to other metal-hydrogen systems. Applying the resulting MLP to study the NQE in the Mg-H system yields new insights with respect to the specific volume, energy, and diffusion rate of hydrogen in this system.

In Materia Computing with Self-organizing Multiterminal Nanowire Networks

Gianluca Milano[2], Fabio Michieletti[1], Davide Pilati[1,2], Carlo Ricciardi[1]
[1]Politecnico di Torino, DISAT, Torino, Italy, [2]Advanced Materials Metrology and Life Sciences Division, INRiM, Torino, Italy

Session 4E: Neuromorphic unconventional and physical computing Symposium, Dobson 4,

February 11 2025, 10:40 - 12:45

In the last few years, there is a growing interest of the research community for self-organizing memristive nanowire networks. Thanks to their structure-function relationship, coupled with nonlinear dynamics and fading memory, such nanonetworks were successfully exploited for brain-inspired computing paradigms, such as physical reservoir computing.

On one hand, using their short-term emergent dynamics, several computing benchmarks were recently accomplished, both static and temporal, such as: MNIST digit recognition [1], speech recognition [2], and Mackey-Glass time series prediction [3]. On the other hand, long-term topological changes can be also induced, similarly to memory encoding consolidation in brain (engram) [4].

The present work aims at better elucidating the link between biological plausibility and computing performance in self-organizing nanowire networks. New results will be also shown about stochastic modelling of nanowire networks and about how multiterminal characterization can give crucial insights on the impact of emergent dynamics and criticality to non-linear transformations.

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Neuromorphic Computing with Physical Neural Networks

Professor Zdenka Kuncic[1]
[1]School of Physics, University of Sydney, Sydney, Australia

Session 4E: Neuromorphic unconventional and physical computing Symposium, Dobson 4,

February 11 2025, 10:40 - 12:45

In response to electrical signals, heterogeneous networks of highly interconnected metallic nanowires exhibit memristive switching, arising from electro-chemical evolution of conductive nano-filaments at their cross-point junctions. Due to their self-organized nature, these physical networks behave similar to disordered many-body physical systems, characterized by emergent nonlinear dynamics such as dynamical phase transitions, synchronization and spatio-temporal correlations. In this talk, we draw a comparison of these emergent dynamics with brain dynamics, arising from neuronal microcircuits established by synaptic connectivity patterns. Using analysis tools and concepts from complexity science and statistical physics, we find a critical threshold at which the emergent dynamics of memristive networks can be identified with symmetry breaking, similar to that exhibited by other complex physical systems, including neuronal networks. Furthermore, we show that this state is optimal for machine learning using physical neuromorphic networks as physics-informed reservoir computers.

Carbon nanotube based multi nanowire memristive switching devices

Natalie Plank[1], Marissa Dierkes, Ned Treacher, Jenna Nguyen
[1]Victoria University of Wellington, Wellington, New Zealand

Session 4E: Neuromorphic unconventional and physical computing Symposium, Dobson 4,

February 11 2025, 10:40 - 12:45

Memristive nanowires have been put forward as a candidate architecture for neuromorphic behaviour on a chip [1], [2], [3], [4]. Combinations of nanomaterials with nanowire morphology allow for simple device patterning and fabrication protocols, where extremely large numbers of junctions can be created and the system probed via mutliple electrical contact points on a single chip.

Here we look at networks of memristive devices based on an underlying network of carbon nanotubes as a physical reservoir systems. We demonstrate device performance improvements with integration of a CNT network with a silver nanowire network [2], [5]. We then investigate the performance of a CNT network scaffolding region with phosphomolybdic acid [6] as switching molecules, as well as extending to other material systems.

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Memristive networks: what's so interesting about them?

Dr Francesco Caravelli[1]
[1]Lanl, Los Alamos, United States

Session 4E: Neuromorphic unconventional and physical computing Symposium, Dobson 4,

February 11, 2025, 10:40 - 12:45

Memristive networks, characterized by their unique ability to dynamically adjust resistance based on the history of current flow, have emerged as a fascinating area of study within nonlinear dynamics. This talk will explore memristive networks' theoretical and practical significance, delving into their complex behavior and potential applications.

The talk will begin with an introduction to the nonlinear dynamics intrinsic to memristive circuits, highlighting the ways in which these networks differ from traditional resistive or capacitive systems and the importance of Kirchhoff's laws for their behavior. We will then explore the theoretical intrigue surrounding these networks, particularly in their emergent properties and dynamic behaviors that offer new insights into complex systems.

A significant focus will be placed on the use of memristive networks as learning devices, specifically through reservoir computing and contrastive learning techniques. These methods leverage the rich dynamics of memristive systems to process information. The discussion will extend to the theoretical capacity of these networks, examining their limits and the possible ways they can be optimized for various tasks.

Multimodal imaging platform to study cartilage degeneration using compression-based depth-resolved polarisation-sensitive optical coherence tomography and vibrational spectroscopy

Dr Frederique Vanholsbeeck[1,2], Mr Darven Murali Tharan[1,2], Dr Marco Bonesi[1,2], Mr Daniel EVERETT[2,4], Dr Matthew Goodwin[1,2], Dr Sue McGlashan[3], Dr Cushla McGoverin[1,2], Dr Ashvin Thambyah[4]
[1]Department of Physics, The University of Auckland, Auckland, New Zealand, [2]The Dodd-Walls Centre for Photonic and Quantum Technologies, Auckland, New Zealand, [3]Department of Anatomy and Medical Imaging, Auckland, New Zealand, [4]Department of Chemical and Materials Engineering, Auckland, New Zealand

Keynote Session 8, Auditorium, February 11, 2025, 13:45 - 14:20

Cartilage tissue is prone to injury and degeneration with age, leading to osteoarthritis (OA), a condition affecting millions worldwide and causing significant pain, disability, and economic burdens. OA patients report late, as aneural cartilage breakdown is painless and end-stage OA results in joint replacement. Understanding the early or pre-OA state of cartilage and the progression of OA is crucial to advancing prevention and treatment strategies. We have made significant progress in developing methods to study early cartilage degeneration efficiently and meaningfully.

We have identified the pre-OA state as a disruption of the cartilage surface layer and a destructuring of the deeper collagen network, subtle changes only detected using microscopy techniques. One key structural feature is the shear discontinuity (SD) that appears under compression as a mechanism to redistribute forces away from the compressed area. Different levels of tissue degeneration can be assessed by SD quantification, which currently requires time-consuming and tissue-destructive methods.

Our team has developed an innovative mechanical testing platform integrating non-invasive real-time imaging, including polarization-sensitive optical coherence tomography (PS-OCT), vibrational spectroscopy, a novel indenter, and displacement sensors. Validated with Differential Interference Contrast and Scanning Electron Microscopy imaging, the compression-based PS-OCT images enable non-destructive dynamic imaging of SD formation during creep loading. Additionally, we register Raman spectra during compression, unveiling the biochemical dynamics within the cartilage. This multimodal platform, developed through collaborative efforts, not only advances our understanding of cartilage biomechanics and degeneration but also paves the way for more effective diagnostic strategies for OA and related conditions.

Advances in Understanding Fundamentals of Memristive Devices Allow New Applications

Professor Ilia Valov[1]
[1]Forschungszentrum Juelich, Juelich, Germany

Keynote Session 9, Dobson 4, February 11, 2025, 13:45 - 14:20

Memristive devices have significantly developed in the last decade, expanding their application horizon much beyond memory applications. Especially important is their functionalities as artificial neurons and synapses, making them promising building units for the next generation bio-inspired neuromorphic hardware. Despite a lot has been learned about materials design and the operation principles of memristors, recent research has shown that fundamentals can still be significantly amended, demonstrating new operation principles and functionalities.

In this contribution, the common electrochemical fundamentals of biological and memristive artificial neurons and synapses will be discussed as well as new aspects on materials design and its influence on the physicochemical processes and resulting functionalities of both ECM (CBRAM) and VCM (OxRAM) devices. The effects of the materials and thicknesses of the capping layer appear of special importance and as well the thicknesses and combination of thicknesses of all involved layers. The selection of different materials is changing the electrochemical nanoionics processes and as well the performance of the memrsitors. For reliable performance the device stack should be considered as a whole, and materials used in the stack and their thicknesses should be coordinated and harmonised.

A special attention will be paid on a new type of application using the quantum conductance levels as standard for resistance in accordance with the new directions given by SI. Justification and the main principle of using the QPC as a standard for resistance will be provided. Different approaches for stabilization of the quantum steps with low number of participating atoms (5 <) will be shown. We introduce the method of electrochemical polishing to ensure stable, reproducible and adjustable contact. Fundamental materials principles and processes will be highlighted.

Demonstration of fermionic time-reversal symmetry in a photonic topological insulator

Dr Lukas J. Maczewsky[2], Dr Bastian Höckendorf[1], Dr Mark Kremer[2], Dr Tobias Biesenthal[2], Dr Matthias Heinrich[2], Dr Andreas Alvermann[1], Professor Holger Fehske[1], Professor Alexander Szameit[2]
[1]Institute of Physics, University of Greifswald, Greifswald, Germany, [2]Institute for Physics, University of Rostock, Rostock, Germany

Session 5A: Photonics and medical spectroscopy, Auditorium, February 11, 2025, 14:25 - 16:00

Much of the recent attention directed towards topological insulators is motivated by their hallmark feature of protected chiral edge states. In fermonic (electronic) topological insulators, these states originate from time-reversal symmetry and allow carriers with opposite spin-polarization to propagate in opposite directions at the edge of an insulating bulk. By contrast, bosonic (or photonic) systems are generally assumed to be precluded from supporting edge states that are intrinsically protected by time-reversal symmetry. Here, we theoretically propose and experimentally demonstrate counter-propagating chiral states at the edge of a time-reversal-symmetric photonic waveguide structure. The pivotal step in our approach is the design and realization of a Floquet driving protocol that incorporates effective fermionic time-reversal symmetry, enabling a photonic version of an electronic topological insulator. Our findings allow for fermionic properties to be harnessed in bosonic systems, thereby offering alternative opportunities for photonics as well as acoustics, mechanical waves and cold atoms.

L. J. Maczewsky, B. Höckendorf, M. Kremer, T. Biesenthal, M. Heinrich, A. Alvermann, H. Fehske, and A. Szameit: Fermionic time-reversal symmetry in a photonic topological insulator. Nature Materials 19, 855 (2020)

Exciton and phase engineering for efficient quasi-2D perovskite light-emitting diodes

Chuanjiang Qin[1]
[1]Chinese Academy of Sciences, Changchun, China

Session 5A: Photonics and medical spectroscopy, Auditorium, February 11, 2025, 14:25 - 16:00

Perovskite light-emitting diodes and lasers are promising for next generation lighting and displays because of their high colour purity and performance. While the management of singlet and triplet excitons is fundamental to the design of efficient organic light-emitting diodes and lasers, the nature of how excitons affect performance is still not clear in perovskite-based devices. In this talk, I will first introduce our new finding that triplet excitons are key to efficient emission in green quasi-2D perovskite devices and that quenching of triplets by the organic cation is a major loss path. Employing an organic cation with a high triplet energy level (phenylethylammonium) in a quasi-2D perovskite based on formamidinium lead bromide yields efficient harvesting of triplets. Furthermore, we observed that upconversion of triplets to singlets can occur, making 100% harvesting of electrically generated excitons potentially possible. The external quantum (EQE) and current efficiencies of our champion green devices reached 12.4% and 52.1 cd/A, respectively. We further improved EQEs over 23% for both green and red devices through phase engineering with extended device operational lifetimes.

Bridging the visible and mid-IR with nano-optics to watch ultrafast vibrational energy cascades

Dr Rakesh Arul[1], Fiona M. Bell[1], Dr. Zhongzheng Yu[1], Prof. Akshay Rao[1], Prof. Jeremy Baumberg[1]
[1]University of Cambridge, Cambridge, United Kingdom

Session 5A: Photonics and medical spectroscopy, Auditorium, February 11, 2025, 14:25 - 16:00

The infrared (IR) spectrum of molecules contains rich structural information, enabling disease diagnosis and greenhouse gas monitoring. Despite such promise, IR detection remains far from democratized due to the costs and limited practical utility of existing technologies. To circumvent this, we take advantage of efficient silicon sensors in the visible to help detect IR, which requires converting IR to detectable visible light. While theoretically proposed by Bloembergen in 1959, realising this conversion has proven challenging due to poor efficiency.

We found that layers of gold nanoparticles, assembled with precise spacing using a dye molecule, possess dual IR and visible plasmon-polaritons, enhancing the local optical field by many orders-of-magnitude. These layers allow conversion of mid-IR light into visible light and the detection down to single molecules. This opens a new area of studying mid-IR fluctuation spectroscopy. Additionally, by placing lanthanide nanocrystals between these layers of gold nanoparticles, mid-IR light can be directly converted into visible light, enabling practical detectors.

Using ultrafast spectroscopy, we measure the vibrational coherence lifetimes of molecules within plasmonic nanogaps, observing a new vibrational cascade mechanism in the formation of collective excitonic states. Measurements of spatio-temporally resolved g(1) correlations via Michelson interferometry reveal the growth of long-range correlations in the formation of a new exciton plasmon-polariton condensate. These observations point to a new kind of room-temperature condensate, only present in plasmonic nanostructures with strong confinement of optical fields, simply created through continuous-wave pumping. This launches new ways of detecting mid-IR light and understanding fundamental light-matter interactions.

Feasibility of Portable Raman Spectroscopy as a Clinical Tool for the Assessment of Photodamage in Skin

Mr Ira Mautner[1,3], Dr Michel Nieuwoudt[2,3], Professor Cather Simpson[1,2,3], Associate Professor Paul Jarrett[4,5]
[1]Department of Physics, The University of Auckland, Auckland, New Zealand, [2]School of Chemical Sciences, The University of Auckland, Auckland, New Zealand, [3]The Photon Factory, The University of Auckland, Auckland, New Zealand, [4]Department of Dermatology, Middlemore Hospital, Counties Manukau Health, Auckland, New Zealand, [5]Department of Medicine, The University of Auckland, Auckland, New Zealand

Session 5A: Photonics and medical spectroscopy, Auditorium, February 11, 2025, 14:25 - 16:00

Raman spectroscopy is a non-invasive technique that has been used to identify biochemical changes associated with chronological and actinic aging. However, laboratory-based equipment is not practical to use as a community-based clinical tool. We are investigating low cost, portable Raman as a tool to rapidly assess biochemical markers of actinic aging in skin. Raman spectra from both UV-exposed skin regions (forehead, cheek, forearm, hand, and shin) and UV-protected regions (behind the ear, and underarms) were measured in 119 participants aged four to ninety-four years old. Exploratory Principal Component Analysis (PCA) was performed on the resulting data set to identify spectral regions attributable to differences in UV-exposure, age, gender, and Fitzpatrick skin type. Synchronous Two-Dimensional Correlation Spectroscopy (2D-COS) was used for higher resolution identification of spectral regions that change with age in UV-exposed and UV-protected skin, as well as to determine how the changes with age at these spectral regions correlate with each other. Asynchronous 2D-COS allowed the relative timings of these changes to be determined for the first time, for both UV-exposed and UV-protected skin. To confirm biological attributions to these spectral regions, Sequential Window Acquisition of all Theoretical Mass Spectra (SWATH-MS) mass spectrometry, along with Raman spectroscopy was performed on skin biopsies from thirteen participants to identify proteins that are significantly differentially expressed in UV-exposed and UV-protected skin, and to relate changes in Raman spectra to changes in the proteome due to long-term UV-exposure.

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Metal-oxide and organic dye-based hybrid flexible printed photodetector for healthcare application.

Ms Swati Suman[1], Mr. PARASURAMAN SWAMINATHAN[1]
[1]Indian Institute of Technology Madras, Chennai, India, [2]Indian Institute Of Technology Madras, Chennai, India

Session 5A: Photonics and medical spectroscopy, Auditorium, February 11, 2025, 14:25 - 16:00

Emerging wearable biosensors have garnered significant interest due to their real-time monitoring and personalized disease diagnostics. Flexible electronics' inherent contortion and stretchability offer several advantages, including replacing costly and cumbersome detection equipment. Optical biosensors and electrochemical biosensors have been developed recently. One of the prominent device structures that is being used is photodiodes. Chemically customized optoelectronic properties and their compatibility with printing processes, organic photodiodes emerge as the best choice. Here, we initially focus on developing a zinc oxide-based hybrid structure for a flexible photodiode. Then, a circuit to process the generated signal is developed to detect the current and measure blood saturation level. The Photodiode is fabricated on a flexible PET-based ITO substrate. The dispersion solution of zinc oxide nanoparticles (NPs) in water is printed on the ITO substrate. Then, it is annealed at 120° C for 60 minutes. Then, a parallel electrode is made by using silver epoxy for contacts. The SQ2 dye is used as red-sensitive material on top of the structure.

We have successfully fabricated a flexible organic dye (SQ2) based hybrid photodiode. The application of organic dye has not been studied yet for flexible electronic and then application for oximeter development. The developed diode showed better sensitivity to the light intensity with a change of 17 nA, & the photo-dark current ratio is twice, and the time response is 1.8/0.7 s as a rise/decay time of under 0.1 V red LED light (18 W/m2). The flexible ITO substrate and printing technique were found suitable for healthcare applications.

Designing light activated biomaterials for tissue engineering and regenerative medicine applications

A/Prof Khoon Lim
[1]University of Sydney, Sydney, Australia

Session 5B: Biomedical and therapeutic materials, Dobson 1, February 11, 2025, 14:25 - 16:00

Biomimicry of native tissue composition and architecture using cell-laden hydrogel constructs is widely recognized as a potential strategy for engineering functional tissue substitutes. Native tissue development (formation and maturation) and homeostasis are dictated by a series of dynamic processes, where cells are presented with physical and chemical stimuli in a spatiotemporally modulated manner. However, current tissue engineering and regenerative medicine strategies have not yet allowed recapitulation of these dynamic processes to fabricate large constructs of clinically relevant sizes. Over the past decades, the field of biofabrication has generated various technologies that enable spatial control over the fabrication of cell-free biomaterials and cell-laden hydrogel-based biomaterials, termed bioinks. This talk will cover the recent published research from my group on applying sacrificial biofabrication approaches to impart high resolution and ordered architecture into large hydrogel constructs, as well as development of novel programmable sacrificial bioinks. Different biofabrication modalities (extrusion, lithography, volumetric) were used, as well as application to various hydrogel-based biomaterials. In additional, a novel gelatin-based sacrificial bioink with delayed dissolution features were developed, allowing spatial and temporal control over introduction of physical architectures into hydrogel constructs. This approach demonstrates the unique capacity of delaying dissolution of sacrificial inks to modulate cell behavior, improving the deposition of mineralized matrix and capillary-like network formation in osteogenic and vasculogenic culture, respectively.

Engineered biomaterials comprises bioactive molecules for surgical sutures potential for wound healing

Prof Azam Ali[1], Ms Christina Deng[2]
[1]Centre for Bioengineering & Nanomedicine, Faculty of Dentistry, Otago University, Dunedin, New Zealand,
[2]Centre for Bioengineering & Nanomedicine, Faculty of Dentistry, Otago University, Dunedin, New Zealand

Session 5B: Biomedical and therapeutic materials, Dobson 1, February 11, 2025, 14:25 - 16:00

Sutures are commonly used in surgical procedures for wounds closure or healing. However, sutures can be potential candidate to deliver drugs directly to wound. Despite the availability of various commercial sutures, none have been designed to effectively distribute drugs with anti-bacterial or anti-inflammatory efficacy. Curcumin, a naturally occurring bioactive compound found in turmeric, displays potent anti-bacterial, anti-inflammatory, and antioxidant properties, making it a promising alternative to synthetic drugs, including antibiotics. In this study we designed an innovative approach and engineered polymeric materials comprising curcumin bioactive and fabricated them into a bioabsorbable surgical suture as a delivery device with great potential for wound healing and tissue regeneration. This research also focuses on the bioengineering concept behind designing and fabricating bioactive microsphere-embedded surgical sutures as a controlled bioactive (drug) delivery system to facilitate wound healing.

Using the universal solid-in-oil-in-water emulsion method, we successfully produced curcumin-loaded microspheres. We measured the particle sizes (34.32 ± 12.82 µm), bioactive loading capacity (12.08%) and encapsulation efficiency (92.43%) of the microspheres, and analysed four different fabrication variables. Afterward, we used melt-extrusion to combine the curcumin-loaded microspheres with bioabsorbable biomaterials polycaprolactone (PCL) and polyethylene glycol (PEG) to create a new surgical suture using 3D printing. These sutures had a smooth surface, exhibited appropriate tensile strength, and were flexible when knotted, meeting the required criteria for surgical sutures. Additionally, this engineered biomaterial suture enabled a sustained and stable release of the bioactive biomolecule, promoting effective wound healing.

Soft conducting polymer hydrogel actuators to study brain cell behavior

Mr Kirill Zhurenkov[1,2], Dr Darren Svirskis[3], Dr Bronwen Connor[4], Dr Jenny Malmström[1,2]
[1]Department of Chemical and Materials Engineering, The University of Auckland, Auckland, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, New Zealand, [3]School of Pharmacy, Faculty of Medical and Health Sciences, The University of Auckland, New Zealand, [4]Department of Pharmacology and Clinical Pharmacology, School of Medical Sciences Faculty of Medical and Health Sciences, The University of Auckland, New Zealand

Session 5B: Biomedical and therapeutic materials, Dobson 1, February 11, 2025, 14:25 - 16:00

The human brain exhibits distinctive mechanical properties, with a soft and dynamic viscoelastic extracellular matrix (ECM) that supports neural cells.1,2 This complexity necessitates advanced materials and techniques for investigating how brain cells respond to mechanical stimuli. In this context, hydrogels are crucial for replicating the brain's ECM regarding chemical composition and mechanical properties. However, traditional hydrogels are static and do not provide dynamic stimulation.3–5 In our study, we developed soft hydrogels based on polypyrrole-poly(N-isopropylacrylamide) (PPy-pNIPAM), which can effectively adjust their mechanical properties through reduction-oxidation (RedOx) processes. These materials closely mimic the brain's ECM, exhibiting Young's modulus values similar to those in the brain. Specifically, the Young's modulus of PPy-pNIPAM hydrogels can be fine-tuned to below 1 kPa, with the ability to RedOx-induce an increase in the Young's modulus from 2 to 4 kPa at 37°C. We also showed that these hydrogels, when modified with RGD peptides, supported the adhesion and survival of cultured SH-SY5Y neuroblastoma cells. Overall, our platform closely resembles the mechanical changes in the human brain following different traumas, such as impact, impulsive, and shock wave loadings,6 providing a promising tool for further in vitro studies involving both normal and tumor brain cells.

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Cellular nanoinjection for biomedical applications

A/Prof Roey Elnathan[1]
[1]Deakin University, Faculty of Health, School of Medicine., Waurn Ponds, VIC 3216, Australia, [2]Monash University, Faculty of Pharmacy and Pharmaceutical Sciences., Parkville campus, Australia

Session 5B: Biomedical and therapeutic materials, Dobson 1, February 11, 2025, 14:25 - 16:00

Cell engineering is a major challenge for translational biomedical research. The key difficulty lies in manipulating cells to transform them without causing irreversible damage or loss of function [1].

Gaining safe, efficient, and non-destructive access to the intracellular environment of diverse cell types holds great promise for the fundamental science and application of intracellular delivery in cell engineering , with significant potential for enhancing human well-being [2,3].

The aim of the talk is to cover the development of engineering novel nanoneedle designs and fabrication paradigms—a transformative shift, allowing precise control of ex-vivo cellular processes, in particular the ability to deliver diverse cargo types via cellular nanoinjection, bringing deep understanding of the fundamental mechanisms at the interface of nanoscale engineering and cellular interrogation [4,5].

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Cobra Venom Factor Prevented Hemodynamic Effects Induced by PEGylated Nanoparticles in a Rodent Model of Acute Hypersensitivity Reaction

Dr Yunn-Hwa Ma[1]
[1]Chang Gung University, Taoyuan, Taiwan

Session 5B: Biomedical and therapeutic materials, Dobson 1, February 11, 2025, 14:25 - 16:00

Polyethylene glycol (PEG)-modified pharmaceuticals can induce acute hypersensitivity reactions (HSR), including complement activation and hypotension, followed by tachyphylaxis with an unknown mechanism. We hypothesized that complement activation by PEGylated nanoparticles induces microvascular occlusion that entrains hemodynamic effects. In anesthetized rats, PEGylated magnetic nanoparticles (PEG-MNPs; iv) with dextran coating induced a temporary, but significant reduction in arterial pressure, renal/cremaster blood flow, and cardiac output, followed by tachyphylaxis and thrombocytopenia. PEG-MNPs (10 mg/kg), but not pristine MNPs, significantly increased renal vascular resistance with a reduction in the cross-sectional area of renal vessels, suggesting microvascular occlusion. In contrast, the vasodilator acetylcholine decreased both blood pressure and vascular resistance before and after administration of PEG-MNP, suggesting an intact endothelium. Complement depletion with cobra venom factor (5 and 20 IU/kg) induced a transient and significant reduction in blood flow and completely blocked PEG-MNP-induced hemodynamic effects (n = 8 and 5, respectively), suggesting an important role for complement activation. Proteomic analysis indicates much higher complement proteins in the hard corona of PEG-MNPs compared to MNPs in plasma from rats; Preexposure of rats to PEG-MNPs or MNPs in vivo greatly reduced plasma proteins with high affinity for PEG-MNPs, which may mediate tachyphylaxis. Therefore, these responses to PEG-MNPs in rats can serve as a model for the study of PEGylated nanocomposite-induced HSR. In conclusion, an increase in systemic vascular resistance is associated with hypotension in HSR induced by PEGylated nanocomposites; complement activation and depletion of complement can trigger hemodynamic responses and subsequently induce tachyphylaxis in HSR.

Catalysing Global Green Hydrogen Production

Professor Antonio Tricoli[1]
[1]The University of Sydney, Australia

Session 5C: Catalysis, Dobson 2, February 11, 2025, 14:25 - 16:00

Hydrogen is emerging as a key player in achieving a carbon-free, environmentally friendly energy future. Its production through water splitting offers a scalable and green solution for storing intermittent renewable energy sources, thereby supporting grid stability and enabling the export of renewable energy to high-demand areas. However, the high cost of noble metal catalysts used in current commercial electrolysers limits both affordability and scalability of hydrogen production. In this presentation, I will discuss advances in multi-scale material design that facilitate the use of low-cost, earth-abundant materials for hydrogen production. I will highlight innovative nanocatalyst synthesis methods that enable roll-to-roll fabrication of anodes and cathodes for alkaline water splitting, achieving enhanced efficiency and stability under industrially relevant conditions. Furthermore, I will explore how these insights can be applied to other environmental technologies, such as CO2 electroreduction and the production of renewable electro-fuels.

Rational Design of Carbon-Neutral Catalysts in Buried Junction Systems for a Sustainable Future

Professor Tae-Hyuk Kwon[1]
[1]Ulsan National Institute of Science and Technologygy (UNIST), Ulsan, South Korea

Session 5C: Catalysis, Dobson 2, February 11, 2025, 14:25 - 16:00

The world is currently confronted with more challenges in the realms of energy and environment, than ever before. In response to these challenges, our group has focused on investigating bias-free buried junction system along with the development of photo/electroactive catalysts for green energy generation, energy recycling, and waste upcycling. This presentation will be divide into three parts: i) molecular design strategy for light-harvesting efficiency, ii) bias-free buried junction system for green energy generation, and iii) carbon-catalysts for eco-friendly environment.

First, vectorial electron transfer in a single organic sensitizer will be introduced by integrating both strong and relatively weak electronic couplings, mirroring the charge separation efficiency seen in natural photosystems to improve light-harvesting efficiency. Next, we have explored the integration of light-harvesting system with catalysts in a monolithic device for a bias-free buried junction system to serve as a power source for H2 or H2O2 generation. This utilizes a platinum-sputtered nickel foil to encapsulate both the dye-sensitized TiO2 layer and the redox mediator electrolyte. This design facilitates spatially controlled cascade charge transfer, effective photo conversion, and water oxidation without the issues of current leakage. Furthermore, our group has conducted research on carbon-catalyst utilizing sonocavitation and nebulization synthesis (SNS) to synthesize frustrated type Lewis acid-base pairs (FLP) doped graphene nanopowder. SNS employs acoustic cavitation, which generates extreme conditions within collapsing bubbles (5000 K and 1000 bar). These unique conditions enable various chemical reactions that are typically inaccessible. We will demonstrate how the utilization of graphitic FLP as catalysts enables the reduction of CO2 and N2, as well as urea production.

Separating Chiral and Catalytic Moieties in MOF Asymmetric Catalyst

Miss Mohana Arul[1]
[1]Massey University, Palmerston North, New Zealand

Session 5C: Catalysis, Dobson 2, February 11, 2025, 14:25 - 16:00

Asymmetric catalysis is a central area of modern chemistry. Applications of MOFs to asymmetric are well established since MOFs offer a platform for substrates to enter the pores, interact with framework components and produce chiral organic compounds via catalysis. Asymmetric catalysis selectively directs the formation of one enantiomer over the other through chiral induction. (1) In conventional asymmetric catalysis, catalytic and chiral elements are tightly linked. In contrast, we have conceptualised an approach known as remote asymmetric induction (RAI). RAI involves the independent compartmentalisation of the catalytic group and chiral element in distinct regions of the catalyst.

Multicomponent MOFs are an ideal platform for the realisation of the RAI concept. We focused on MUF-77 (2) (Massey University Framework), composed of three distinct organic linkers connected by a Zn4O secondary building unit. In MUF-77 analogues, we have successfully installed catalytic units and chiral elements on separate framework linkers. Specifically, two linear linkers frame the same pore environment, creating a confined active site. Substrates enter these framework channels, interact with the catalytic unit, and are oriented by the chiral element through noncovalent interactions, resulting in chiral induction.
We report the successful implementation of the RAI concept in MUF-77 analogues to carry our organic transformations with high enantioselectivity. Our goal is to achieve over 90% enantiomeric excess (ee) by systematically exploring a broad range of catalytic units and chiral elements. This will require extensive screening across diverse reactions with different reactants to identify the most effective combinations for maximizing ee.

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Extraordinary performance of a platinum-copper dual single atom electrocatalyst for the selective oxidation of 5-hydroxymethylfurfural to 2,5-furandicarboxylic acid

Dr Yongfang Zhou[1], Miss Yan Liu, Dr Yu Mao, Prof Ziyun Wang, Prof Geoffrey I. N. Waterhouse, Prof Yi Shen
[1]University Of Auckland, AUCKLAND CENTRAL, New Zealand, [2]South China University of Technology, Guang Zhou, China

Session 5C: Catalysis, Dobson 2, February 11, 2025, 14:25 - 16:00

Electrochemical oxidation of biomass-derived 5-hydroxymethylfurfural (HMF) offers a promising pathway towards many high-value chemicals. However, selective oxidation of HMF to specific products is still challenging. Herein, we report the selective electrocatalytic oxidation HMF to 2,5-furandicarboxylic acid (FDCA) in alkaline media over Pt-Cu dual single atom sites immobilized on nitrogen/sulfur co-doped carbon nanosheets (PtCu/NCNSs). The compositionally-optimized Pt2Cu1/NCNSs catalyst exhibits extraordinary performance for the HMF oxidation reaction (HMFOR) in terms of a low onset potential (0.98 V), large current density (1006.4 mA mg-1 at 1.42 V), high FDCA yield (97.4%), and high Faradaic efficiency (97.6%), outperforming most catalysts reported in the literature. A reference Cu/NCNSs catalyst showed a high selectivity towards 5-formyl-2-furancarboxylic (FFCA) (yield 81.6%) rather than FDCA. Experimental and theoretical studies reveal that Pt single atom sites adsorb OH*, thereby promoting the deeper oxidation of HMF to FDCA. HMF molecules adsorb on the Cu single atom sites are then oxidized by adsorbed OH* on the Pt single atom sites. This study guides the rational design of highly selective electrocatalysts for HMF oxidation to specific products.

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Unique Liquid Metal Activation Pathways with Applications for Renewable Fuels

Dr Mariam Ameen[1], Mujtaba A. Juddy[1], Fahad Jabbar[1], Mehmood Irfan[1], Pierre H. A. Vaillant[1], Caiden J. Parker[1], Dr Karma Zuraiqi[1], Dr. Ali Zavabeti[2], Dr Vaishnavi Krishnamurthi[1], Dr Andrew J. Christofferson[1], Professor Salvy P. Russo[1], Dr. Nastaran Meftahi[1], Dr Ken Chiang[1], Dr. Torben Daeneke[1]
[1]RMIT University City Campus, Melbourne, Australia, [2]University of Melbourne, Melbourne, Australia

Session 5C: Catalysis, Dobson 2, February 11, 2025, 14:25 - 16:00

Post-transition-based liquid metals are promising catalysts due to their high reaction rates, excellent deactivation resistance, and tuning potential, which form intermetallic and interfacial compounds through alloying with noble and transition metals.[1, 2].The mechanism by which alloyed metals enhance activity is currently unknown and debated, with some suggesting they act as single atom catalysts[3] and others activating the liquid metal particularly gallium[4].Herein, we report the synthesis of liquid metal alloys consisting of atomically dispersed Cu in the eutectic gallium-indium alloy (or EGaIn) and investigate the role Cu plays in the activation of Ga. The morphology of the synthesized alloys was studied using SEM analysis while the interface was examined using XPS. These surface studies revealed that the Cu was evenly distributed in E-GaIn alloys in contrast to Ga based liquid metal alloys. The performance of Cu-based liquid metal alloys was assessed for solketal synthesis. The open circuit potential of Cu-EGaIn was found to be -0.298 V vs SHE, comparable to a conventional reducing agent NaBH4. Molecular dynamics simulations indicated that the activation of Ga atoms by adjacent Cu atoms is responsible for the observed enhanced activity of the Cu-EGaIn alloy in a series of reduction reactions, including the organic acetalization reaction, inorganic reduction of triiodide, and hydrogen production. Cu catalyzes gallium oxidation in liquid metals, supporting the hypothesis that small amounts of alloyed transition metals can activate gallium atoms in liquid metals. This research highlights opportunities for the use of liquid metals as reducing agents in organic synthesis and hydrogen on-demand applications.

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New Wool-Derived Materials for Pollutant Gas Absorption

Dr Amy Cruickshank[1], Mrs Gail Krsinic[1], Mrs Claire Clark[1], Mr Ben Edwards[1], Dr Rob Kelly[2]
[1]Lincoln Agritech Limited, Lincoln, New Zealand, [2]Wool Source Limited, Christchurch, New Zealand

Session 5D: Waste to value, Dobson 3, February 11, 2025, 14:25 - 16:00

Increasing global air pollution levels caused by urbanisation, industry and transport is recognised as a major public health concern with the World Health Organisation (WHO) reporting that, in 2019, 99 % of the world population was living in places where the WHO air quality guidelines and limits were not met.[1] Natural wool fibres are a sustainable, renewable and biodegradable resource and are well known to bind and neutralise pollutant gases such as NO_2, SO_2, and formaldehyde in urban environments due to their unique protein composition.[2] As part of the 'New Uses for Wool' research program, our work has focused on deconstructing coarse wool fibres to create new wool-derived material formats (e.g., powders, pigments and cortical cells) that contain the inherent performance benefits of wool but can be used in new application areas not previously accessible for wool fibres. This presentation will discuss the pollutant gas absorption performance of the new wool-derived materials and their functionality as anti-pollution additives in new application areas, such as personal care[3] and filtration, currently being commercialised by Wool Source.[4] It will be shown that these novel wool-derived materials have high surface area and a rich array of surface chemical groups available to bind and neutralise pollutant species. A mechanism of action based on the antioxidant and free-radical scavenging capabilities of the wool-based products will also be discussed.

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Novel cellulose fibres from whole plant material

Dr Helen Ashmead[1], Mr Shaahin Saleh[1], Mrs Erica Sue-Tang[1], Dr Rob Kelly[1]
[1]Lincoln Agritech Ltd, Christchurch, New Zealand

Session 5D: Waste to value, Dobson 3, February 11, 2025, 14:25 - 16:00

Textiles produced from biodegradable fibres are an attractive alternative to synthetics. While the end product appears to be more sustainable, the methods used to produce biodegradable fibres, such as man-made cellulose fibres (MMCF), can be environmentally damaging in a myriad of ways.

- High energy usage and pollutant production
- Release of toxic chemicals into the air and water ways
- Limited cellulose feed stock leading to habitat destruction through deforestation
- Extensive byproducts from wood processing not used in fibre production

Research is underway, supported by the New Zealand Government Endeavour Fund, examining the potential for extruding fibres from plant material that has minimal processing and thus minimizes byproducts and incorporates non cellulose materials into cellulosic fibres. Novel characteristics such as colour and fragrance arise from the non-cellulose components retained in fibres.

Producing MMCF from whole plant material broadens the cellulose feedstock as less purity is needed. Mātauranga Māori (Māori traditional knowledge) related use of New Zealand native plants has guided the choice of sustainable, native cellulose source material. This research shows the potential for a completely new, and environmentally friendly path towards generating cellulose fibres for the textile industry.

Key Words: Cellulose, textiles, sustainability, cellulosic fibres, Mātauranga Māori

A Zero-Liquid-Discharge Method for Cleaner Vanadium Recovery Using Volatile Reagents

Mr Aston Pearcy[1], Professor Aaron Marshall[2], Professor Chris Bumby[1]
[1]Paihau-Robinson Research Institute, Victoria University of Wellington, Lower Hutt, New Zealand,
[2]University of Canterbury, Christchurch, New Zealand

Session 5D: Waste to value, Dobson 3, February 11, 2025, 14:25 - 16:00

Vanadium is a 'critical metal' with significant applications in the metallurgical and chemical industries. Natural vanadium occurrence is highly dispersed and is generally found at low grades.[1] Hence, most of the world's vanadium is extracted from by-product slags produced during steelmaking, which have heavily upgraded values of vanadium relative to natural sources.[2]

Vanadium is often present in slags as the V(III) ion. Recovery methods typically produce V(V) via oxidative roasting, before leaching in an aqueous lixiviant solution.[3] The subsequent leachate solution of V(V) ions is subjected to an 'ammonium-salt' precipitation, where a large excess of an ammonium salt is added to precipitate vanadium as an ammonium vanadate.[4] This process discharges a huge amount of saline, ammoniated wastewater to the environment.

Here, we report a new, cleaner, vanadium precipitation method. We have found that a reductive precipitation using a volatile reductant can produce solid vanadium-bearing material. This method is cleaner than conventional industrial methods, whilst still reaching comparable precipitation efficiencies and product purity. As the reductant and its by-products are volatile, heat can be applied to remove them from the system. Therefore, the leftover solution after reduction can be recycled to the leaching step, making this a Zero-Liquid-Discharge Process.

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Sustainable approach to recover and recycle critical materials from Lithium ion waste batteries

Miss Thilini Lakshika Rathnayaka Mudiyanselage[1], Mr Dmitri Golberg[1], Mr Deepak Dubal[1]
[1]School of Chemistry and Physics and QUT Centre for Materials Science, Queensland University of Technology (QUT), Brisbane, Queensland 4000, Australia, Brisbane, Australia

Session 5D: Waste to value, Dobson 3, February 11, 2025, 14:25 - 16:00

The rising global demand for lithium-ion batteries, fueled by electric vehicles, electronics, and renewable energy storage, has increased concerns over battery disposal's environmental impact. Despite the increasing need for lithium-ion batteries, there is a shortage of critical materials required for their production. Recycling offers a potential solution, but current methods are inefficient, producing high emissions and hazardous waste, highlighting the need for improved technologies. This research focuses on developing a sustainable process for selective extraction of essential materials from battery waste using deep eutectic solvents (DES)1, followed by their characterization and repurposing in high-value applications, such as anode and cathode materials. Industrial black mass samples were utilized, and various analytical methods were used for characterization. Graphite was recovered using the froth flotation method, while DES, particularly a choline chloride: ethylene glycol mixture, was used to leach Ni, Mn, Li, and Co under different pH conditions. The leached solutions were filtered, dried, and further characterized. The recovered materials were adjusted to an 8:1:1 NMC ratio using a co-precipitation technique to produce NMC cathode materials, while the recovered graphite was repurposed for anode production. The performance of the fabricated batteries was tested using electrochemical techniques. The results of this research demonstrate the efficient and environmentally friendly recovery of critical materials from used lithium-ion batteries. The recovered materials are expected to produce NMC cathodes with specific capacities ranging from 150-200 mAh/g, comparable to new NMC materials, and graphite anodes with capacities around 300 mAh/g.

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Analog Behavior in Oxide-Based CBRAM/ECRAM

Dr Michael Kozicki[1], Professor Matthew Marinella[1], Mr Resalat Faruque[1], Mr Smitha Swain[1], Mr Quinn Nguyen[1], Mr Keonwon Beom[1]
[1]Arizona State University, Tempe, United States

Session 5E: Neuromorphic unconventional and physical computing Symposium, Dobson 4, February 11, 2025, 14:25 - 16:00

Resistance switching in metal-oxide-metal structures, including metal cation-based Conductive Bridging Random Access Memory (CBRAM), has been studied for decades, particularly in the context of memory and data storage applications [1]. Cation switching involves the transport and reduction of metal ions from an oxidizable anode to form a highly conducting metallic filament in the insulating oxide, and this results in a dynamic resistance range of many orders of magnitude. A bias opposite to that which forms the filament is used to dissolve it and reduce the excess ions, thereby returning the device to its high resistance state. Although memory applications typically demand discrete resistance levels, these structures are also capable of producing continuous changes in both resistance and capacitance, a property that has potential applications ranging from electronic trimming in analog integrated circuits to neuromorphic computing [2]. This talk will present results from a range of device types, including two- and three terminal structures, and will describe the mechanisms behind the continuous changes in their resistance and capacitance. We will focus on analog behavior in oxide-based ion conductors due to their compatibility with CMOS process flows, including silicon suboxide (SiOx, where x is around 1.3) in vertical devices, copper oxide/tungsten oxide bilayers in lateral devices [3], and Cu/SiOx/WOx in three-terminal electrochemical memory (ECRAM). Applications of these materials and devices in neuromorphic applications will be highlighted as part of the discussion.

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Creation of various functions and improvement of the device performance by means of ionic nanoarchitectonics

Dr Kazuya Terabe[1], Takashi Tsuchiya[1], Tohru Tsuruoka[1]
[1]National Institute for Materials Science (NIMS), Tsukuba, Japan

Session 5E: Neuromorphic unconventional and physical computing Symposium, Dobson 4, February 11, 2025, 14:25 - 16:00

The properties of materials at the nanoscale are strongly influenced by small changes in the arrangement and composition of their constituent atoms. We have extensively studied unique nanophenomena arising from the atomic-scale control of arrangement and composition at heterointerfaces of functional materials [1-3]. Ionic nanoarchitectonics method enables such atomic-scale interface control by exploiting local and reversible ion transport and electrochemical phenomena in solids. By controlling the heterointerfaces of different functional materials, different nanophenomena can be created. The unique properties resulting from these phenomena can be used to create a variety of devices with electrical, magnetic, optical and other functions [4]. To date, we have used the ionic nanoarchitectonics to create some devices with diverse functions and superior performance to improve conventional electronic devices. These include atomic switches, decision-making devices, artificial synaptic devices, all-solid-state electrical double-layer transistors, on-demand multifunctional devices, magnetisation tuning devices and so on [1-4]. In particular, this ionic nanoarchitectonics is a promising method for fabricating artificial intelligence (AI) devices based on neuromorphic properties, which have attracted much attention recently, and is expected to contribute to the development of next-generation hardware-oriented AI technology.

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Two-dimensional materials for next-generation electronics and optoelectronics technologies

Professor Sumeet Walia[1]
[1]RMIT University, Melbourne, Australia

Session 5E: Neuromorphic unconventional and physical computing Symposium, Dobson 4, February 11, 2025, 14:25 - 16:00

Atomically-thin materials possess unique intrinsic properties and are amenable to a range of tuning techniques. We harness these properties underpinned by application demand and work with industry to translate into end-user products.

Firstly, we synthesise a variety of atomically-thin metal oxides, mono/dichalcogenides and elemental 2D materials using solid, liquid and vapour phase techniques guided by application.

Our fundamental advances have been uncovering the origins of oxidative degradation in few-layer black phosphorus (BP) and subsequently proposing an ionic liquid-based approach to prevent ambient degradation of BP. Using defect engineering, we have demonstrated neuromorphic vision and processing sensors. We have explored the use of hybrids of dissimilar materials to enhance electronic and optical performance. Ultra-thin layers have been used to develop one of the world's thinnest photodetectors that can sense all shades of light from UV-infrared. We further study strain-tunability in low-dimensional structures via integrating them onto elastomeric platforms.

Using a cross-disciplinary approach, we deploy multifunctionality of these new material systems into solving technological challenges for industry partners across sectors that require novel materials and functions to be integrated into their products.[1-5]

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Acoustically Levitated Droplets as Advanced Materials

Professor Geoff Willmott[1,2], Zhifei Geng[1]
[1]University Of Auckland, Auckland, New Zealand, [2]The MacDiarmid Institute, Wellington, New Zealand

Session 6A: Nano and micro mechanical control, Auditorium, February 11, 2025, 16:30 - 18:10

Nucleation, growth, and shrinkage of liquid aerosol drops are heat-induced processes with broad relevance for sustainability. They are also critical processes within fields as important and diverse as disease transmission, climate modelling, and production of milk powder via spray drying [1]. However, liquid micro- and nanoparticles dispersed in air are usually studied collectively (e.g. via light scattering) or in contact with a surface. Acoustic levitation [2-4] is a relatively facile and flexible way for detailed study of individual droplets in air. This presentation will introduce this method via a study of simple and complex fluid droplets. While water drops can be expected to dry at a rate that is consistently linear with respect to surface area [2], complex fluids are much less straightforward, with phenomena such as buckling being observed as solid residues form [5]. The presentation will also discuss a variety of interesting experimental topics arising while developing a new acoustic levitation rig. These include droplet imaging, control and measurement of temperature and humidity, suppressing the effect of the acoustic field, and extensions towards impact experiments and nanoscale sampling.

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Stroking Through Electrolyte: Liquid Metal Droplet Propulsion Through Pulse Time Modulation

Mr Richard Fuchs[1], Dr. Jianbo Tang[1], Prof. Kourosh Kalantar-Zadeh[2], Prof. Guangzhao Mao[1], Prof. Michael D. Dickey[3], Dr. Mohamed Kilani[1], Dr. Shiva Abdoli[1], Mrs. Ruohan Yu[1], Mrs. Nur-Adania Nor-Azman[2], Dr. Shi-Yang Tang[3]
[1]University of New South Wales (UNSW), Kensington, Australia, [2]University of Sydney, Darlington, Australia, [3]University of Southampton, Southampton, United Kingdom, [4]North Carolina State University, Raleigh, USA

Session 6A: Nano and micro mechanical control, Auditorium, February 11, 2025, 16:30 - 18:10

Active droplets play important roles in microfluidics, robotics, and micro-electromechanical systems. As a special class of active droplets that are conductive, reactive, and of high surface tension, liquid metal droplets (LMDs), specifically those made of gallium and its alloys, can be driven by electric-field-induced surface (Marangoni) flows to function as reconfigurable components in actuators, sensors, catalytic reactors, and antennas. When immersed in an electrolyte medium, stimulating LMDs using an electric field induces concurrent electro-hydrodynamic flows and electrochemical surface oxidation (passivation). It is however difficult to decouple these two effects which brings complexity in controlling LMD motions. Highly effective propulsion is often seen in biosystems. For instance, fish and jellyfish are excellent swimmers, and they both use undulated body locomotion to propel themselves through water at high speeds and low energy consumption. Inspired by such undulating bio locomotion, here we introduce a pulse time modulation (PTM) strategy, in an electrochemical setting by propelling the LMDs forward during the voltage-on phases and facilitating surface recovery from oxidation during the voltage-off phases. Counterintuitively, by taking such intermittent 'rests', the LMDs effectively inhibit the unfavourable impact of oxidation, granting high motion controllability. Combining high-speed imaging, motion tracking, machine learning, and electrochemical analysis, we show how electro-hydrodynamic flows and surface oxide formation/dissolution interplay to generate well-defined motion regimes. A quasi-analytical model further describes droplet motions and a rotary LMD motor showcases the versatility of our approach. This work provides the fundamental framework and viable strategy for designing innovative liquid metal-based systems.

From Movie Screen To Science: Bringing Big Hero Six's Reconfigurable Approach To The Microscale

Mr Nicholas Carlisle[1], Dr Volker Nock[1], Dr Catherine Whitby[2], Dr Jack Chen[3], Dr Ebubekir Avci[1]
[1]University of Canterbury, Christchurch, New Zealand, [2]Massey University, Palmerston North, New Zealand, [3]Auckland University of Technology, Auckland, New Zealand

Session 6A: Nano and micro mechanical control, Auditorium, February 11, 2025, 16:30 - 18:10

Swarm (collective behaviour) is a phenomenon found throughout the natural world, where groups come together to complete tasks that an individual cannot. This behaviour has long been an inspiration in the field of microrobotics with many potential applications, including biomedical, micromanufacturing, manipulation [1]–[3]. Robotics at this scale comes with a range of its own challenges, often leading to the need for highly tailored robots manufactured for single use applications. Alternatively, using a large number of simple robots with swarm like capabilities offers a reconfigurable and flexible approach for many complicated tasks. Swarm microrobotics use external stimuli to induce and control the self-assembling behaviour of particles (microrobots) [4], with control of these swarms limited in terms of application requirements unique to their external stimuli. Optical force-induced assemblies are made by optical tweezers (OT) trapping a particle at an interface (i.e. glass-liquid) attracting and accumulating nearby particles. Our previous work [5] was the first to use the OT manipulation and automation capabilities, investigating assembly, locomotion and studying assembly-assembly interactions. Here, we further this work by developing higher level manipulation and automation control techniques over these robotic assemblies. Additionally, we introduce a novel idea of using DNA strands as a form of flexible mechanical bonding between robots in an assembly, thus developing a unique form of micro-manufacturing that can easily be disassembled back to its original building blocks.

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Tiny Robots: A Giant Step Towards Managing Gut Health

Mr Adam Carlisle[1], Dr Volker Nock[1], Dr David Thomas[2], Dr Ebubekir Avci[1]
[1]University Of Canterbury, Christchurch, New Zealand, [2]Massey University, Palmerston North, New Zealand

Session 6A: Nano and micro mechanical control, Auditorium, February 11, 2025, 16:30 - 18:10

The microbiota within the human gut has recently shown its importance in the early diagnosis of metabolic diseases including cancer, type-2 diabetes, and obesity, as well as effecting mood and behaviour [1-3]. However, no available clinical method exists to sample this microbiota from the small intestine without either contamination or high levels of invasiveness [4]. Hence, our group developed a prototype swallowable robotic capsule which successfully scraped 100 µL of microbiota from the wall of a living segment of a small intestine [4]. To be suitable for human use, the capsule size needs to be reduced from 45 mm x Φ12 mm to 32 mm x Φ 12 mm [4]. Currently, the actuation of the sampling mechanism is effective, but it requires a large space within the capsule. Hence, further miniaturisation of the actuation mechanism is required to reduce the size of the capsule. In the current prototype, a 2-way shape memory alloy (SMA) spring is utilised to open and close the sampling door on the outside wall of the capsule. This method using an SMA spring has proven to be effective, therefore, the current work considers alternative layouts, and uses of SMA materials to miniaturize the sampling mechanism. In the future, this miniaturised sampling mechanism will bring robotic capsules closer to clinical use, where lives can be saved through early diagnosis of metabolic diseases.

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Squeezing Through the Gut: Micro-Manufacturing of Smart Capsule

Mr Martin Allen[1,2,3], Dr Ebubekir Avci[2,3], Dr Volker Nock[2,3]
[1]Massey University, Palmerston North, New Zealand, [2]University Of Canterbury, Christchurch, New Zealand, [3]MacDiarmid Institute, Wellington, New Zealand

Session 6A: Nano and micro mechanical control, Auditorium, February 11, 2025, 16:30 - 18:10

Capsule robots are small ingestible devices which can perform wireless operations within the human Gastro-Intestinal (GI) tract. Since 2000, wireless capsule endoscopes have been used to inspect difficult to reach areas within the small bowel, with less invasiveness [1]. Recently, there has been interest in expanding the functionality of these devices to perform more complex operations like drug delivery [2], sampling, and biopsies [3]. Current capsule robot prototypes feature advanced robotic mechanisms which can extract samples through sharp needle biopsy or by scraping mucus off the intestinal lining. These advanced designs require more power, control, and physical mechanisms confined within the capsule, in turn requiring more space than traditional endoscopic capsules due to miniaturisation of components not keeping pace [4,5]. Across literature, most capsule designs use the same materials and shapes, but this may not be the best way to transit through the gut. In this project, several alternative designs involving patterned surfaces using different materials (FHD-1200 printer resin and Ultra-high-molecular-weight polyethylene (UHWMPE)) and manufacturing methods (Printing and Machining) have been used. We will show testing of these designs using a silicone intestinal model to measure the force required to transit difficult areas of the gut, and a robotic model which simulates intestinal peristalsis to measure the capsule performance when subjected to peristaltic forces.

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Improving the size and safety of microbiota sampling capsule robots

Mr Angus Quigley[1], Dr Volker Nock[1], Dr David Thomas[2], Dr Ebubekir Avci[1]
[1]University of Canterbury, Christchurch, New Zealand, [2]University of Massey, Palmerston North, New Zealand

Session 6A: Nano and micro mechanical control, Auditorium, February 11, 2025, 16:30 - 18:10

When analysed, the microbiota found in the Gastrointestinal (GI) tract can help to develop an understanding of the state of health of an individual under examination [1]. In practice, there are a limited number of methods available to sample microbiota from the GI tract. Of these, the non-invasive sampling methods are ineffective as they sample faeces rather than the microbiota itself [2]. Moreover, invasive sampling techniques are also difficult to perform and can put the individual under examination in a hazardous environment [2]. A better way to sample microbiota from the GI tract is to use a non-invasive sampling capsule robot that can extract microbiota from different locations in the tract [3]. Our research team has successfully developed a robotic capsule concept to achieve this task [4]. The capsule measures 45 mm x ϕ 12 mm, which is not appropriate for human trials, and only suitable for large animals [4].

The robot needs to measure less than 32 mm by ϕ 12 mm to be suitable for human trials [4]. Removing the battery and complex electronics, and controlling the device using external magnets would allow the capsule to be reduced in size, while also removing a potentially dangerous battery from inside an individual under trial [5]. We will aim to show that the sampling actuation mechanism can be operated magnetically, eliminating the need for power-consuming electronics within the capsule robot. This would result in a safer device for human consumption.

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He Honoka Hauwai / German-New Zealand Green Hydrogen Centre for Research, Networking and Outreach

Professor Sally Brooker[1], Dr Paul Jerabek[2]
[1]University Of Otago, Dunedin, New Zealand, [2]Institute for Hydrogen Technology, Helmholtz Zentrum Hereon, Geesthacht, Germany

Session 6B: Collaboration and engagement, Dobson 1, February 11, 2025, 16:30 - 18:10

Climate change requires:
(a) Reduction in energy consumption, for example by improving house insulation standards and public transport.
(b) Rapid increase in renewable electricity generation and a range of storage options (to cover intermittency of generation).
(c) Rapid replacement of our present range of carbon-emitting fossil fuels (coal, oil, natural gas) by a suite of carbon-zero and carbon-neutral fuels. The best carbon-zero fuel is direct electrification (from renewable generation), followed by batteries and green hydrogen (two options to store renewable energy) depending on the niche use case.
(d) Conversion of existing heavy emission chemical industry processes to lower emissions options. For example, the use of green rather than grey hydrogen in ammonia and methanol production.

An overview of the place of green hydrogen as a key industry chemical, as well as in the suite of future fuels, will be presented, followed by an introduction to He Honoka Hauwai and to our German-NZ-wide team’s activities.

Towards A Green Industry Sector: Decarbonising the Industrial Sector in Germany and Cooperation Potential with New Zealand

Ms Franziska Teichmann[1]
[1]adelphi, Sydney, Australia

Session 6B: Collaboration and engagement, Dobson 1, February 11, 2025, 16:30 - 18:10

The decarbonisation of the industry sector is crucial to the achievement of national climate targets and hence of the Paris climate goal more broadly. Germany seeks to reach carbon neutrality in 2045, New Zealand in 2050. The comparative study by adelphi and the German-New Zealand Chamber of Commerce identifies key levers for accelerating industrial decarbonisation efforts in both countries and makes suggestions for bilateral cooperation on these key challenges.

Practical educational resources co-created with Mātauranga Māori and Pacific knowledge to empower a new generation of community scientists

Dr Matthew Cowan[1], Dr Matthew R. Wilkins[2], Stephanie Rapciak[2], Dr Madelyn Leembruggen[2], Ashalyna Noa[1], Garrick Thorn[1], Shallu Verma[1], Christina Howat[1]
[1]University Of Canterbury, Christchurch, New Zealand, [2]Galactic Polymath, Minneapolis, USA

Session 6B: Collaboration and engagement, Dobson 1, February 11, 2025, 16:30 - 18:10

This presentation highlights fantastic freely-available educational modules combining science, engineering, Mātauranga Māori, and Pacific knowledge for high school students. [1, 2]

The importance of STEM education in empowering communities is acknowledged by the New Zealand government through the Curious Minds programme, which funds work to boost engagement between science, technology and society. Curious Minds encourages all New Zealanders to ask good questions, solve local problems and uncover innovative science and technology solutions for a brighter future.

We present two examples of educational modules created for high schools students and provide a generalized framework and principles to help audience members create their own educational resources.

Pacific H2O is the first module, focused on case studies and examples of providing clean water in Pacific Nations. The highlight of this module is an interactive choose-you-own adventure lab, which sees students form teams to investigate and treat water samples from three island water sources. The lab experience is supported by engagement activities, science and engineering concepts, and cultural context and narratives.

Colourful Solutions is the second module, focused on the value of colour to society and how that colour is procured. This module focuses on the concepts of scalable and sustainable production, with connection to Mātauranga Māori, indigenous dye production, and the cultural context of colour.

1. Colourful Solutions. https://www.galacticpolymath.com/lessons/en-US/4

2. Pacific H2O. https://www.galacticpolymath.com/lessons/en-NZ/13

Protein reconfiguration and adsorption at the oil-water interface

A/Prof Catherine Whitby, Mr Braydon Nikolaison
[1]Massey University, Palmerston North, New Zealand

Session 6C: Proteins and micelles, Dobson 2, February 11, 2025, 16:30 - 18:10

The mechanical properties of protein layers at oil-water interfaces have a central role in the stability and flow behaviour of food emulsions.1-3 Protein molecules are thought to diffuse to, and re-orientate at, the boundary between the polar and non-polar phases. The molecules unfold and become entangled, forming a gel-like network. The structural changes that occur during layer formation, and hence their impact on the layer elasticity, remain poorly understood.

We investigated the impact of conformational changes to β-lactoglobulin molecules in solution on their behaviour at the oil-water interface. Protein behaviour was compared at interfaces with oils of the same hydrocarbon chain length, but different polarity. Changes in the protein secondary and tertiary structure were caused by chemical denaturants, or by heating. We used pendant-drop tensiometry, and double wall ring interfacial rheology, to probe the properties of the interfacial layer formed by the modified protein.

Our key finding is that unfolding β-lactoglobulin in solution can enhance the elasticity of the interfacial layer. Adsorption of native proteins is typically slow at interfaces between aqueous solutions and polar oils. Adding guanidine hydrochloride to aqueous protein solutions causes the protein to reconfigure its globular structure to expose more hydrophobic residues. The changes enhance the rate of formation of interfacial layers from solutions of unfolded proteins onto polar oils. These findings provide insights into the role of protein denaturation at interfaces in stabilisation of food emulsions.

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Lipid-sealed microchambers with integrated ion-sensing transistors - A new tool for membrane protein studies.

Mr Shuji Kojima[1], Dr Siddharth Rawat[1,2], Prof. Hiroyuki Noji[3], A/Prof. Lawrence Lee[2], Professor Adam Micolich[1]
[1]School of Physics, University of New South Wales, Sydney, Australia, [2]School of Medical Science, University of New South Wales, Sydney, Australia, [3]School of Engineering, University of Tokyo, Tokyo, Japan

Session 6C: Proteins and micelles, Dobson 2, February 11, 2025, 16:30 - 18:10

A central endeavour in bioelectronics is the development of new devices for transducing ionic signals into electronic signals and vice versa. This presents some particularly interesting challenges that span from the development of capabilities for new materials with high ionic conductivity or strong electronic-ionic interactions to novel applications such as medical diagnostics.

We report the development of a PEDOT-PSS transistor based platform to enable the simultaneous electrical and optical study of membrane proteins down to the single protein level. This system featuring PEDOT-PSS organic-electrochemical transistors built into a glass-bottomed attolitre volume well, sealed with lipid bilayer, is currently being tested using the passive pore alpha-hemolysin, but could be extended to other active pores, e.g., ATPase or rhodopsin, and combined with proton-transporting materials (e.g., Nafion) for more building complex iontronic systems.

Reconfigurable Pickering Emulsions

Miss Shivangi Chourasia[1], Assoc. Prof Catherine Whitby[1]
[1]Massey University, Palmerston North, New Zealand

Session 6C: Proteins and micelles, Dobson 2, February 11, 2025, 16:30 - 18:10

Reconfigurable emulsion systems have emerged as a growing field in colloidal science, offering the ability to control the stability and functionality of emulsions. These systems exhibit responsiveness to external stimuli, allowing for adaptive reconfiguration of the emulsion shape and structure in response to environmental conditions. Advances have been made in developing complex emulsion systems that can controllably be altered after emulsification by stimuli such as temperature, pH, magnetic field and light.1–3 However, using particles for stabilising these complex emulsion systems remains a critical area requiring investigation and understanding.

Reconfigurable emulsions are colloidal systems consisting of two or more immiscible liquids stabilised by particles or stimuli-responsive surfactants or a combination of both. We have prepared an oil-in-oil-in-water double emulsion using hydrocarbon and fluorocarbon oils.4 To stabilise the interfaces within this system, we used dimethylsiloxane surface-modified hydrophobic silica particles further functionalised with fluorophilic groups to stabilise the oil-oil interface and sodium dodecyl sulphate to stabilise the oil-water interface. Our research extends the previous findings 4 by exploring how a change in the degree of fluorination of the particles or using oils with different dielectric constants impacts the emulsion configuration. We also investigated how the emulsion behaves with temperature variations.

We are using optical microscopy and confocal microscopy to visualise the changes in the droplet shape and morphology. Altering the polarity of hydrocarbon oils causes the droplet morphology to transition from a nested droplet configuration to a Janus-type arrangement. This transformation can be attributed to an increase in oil-oil interfacial tension with the increase in dielectric permittivity of the hydrocarbon oils.5 As the temperature increases above the upper consolute point, the hydrocarbon and fluorocarbon oils merge into a single phase. Intriguingly, subsequent cooling of the emulsion leads to the formation of multiple droplets of one oil ensconced within the confines of the other oil. Our overall goal is to design and develop complex Pickering emulsion systems that can respond to stimuli like pH, light, temperature and magnetic fields by reconfiguring in a controlled manner.

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Micelles Based Synthesis of 2D and 3D Covalent Organic Frameworks Using Surfactants.

Ms Sri Varshini Murugan[1]
[1]Victoria University of Wellington, Wellington, New Zealand

Session 6C: Proteins and micelles, Dobson 2, February 11, 2025, 16:30 - 18:10

Covalent Organic Frameworks (COFs) are a class of highly crystalline, porous networks that excel in energy conversion and storage applications, such as photocatalysis, water splitting, and supercapacitors. Their exceptional properties—including high surface area, thermal stability, tunable pore sizes, good electrical conductivity and mechanical strength. However, conventional COF synthesis methods often yield materials with suboptimal crystallinity, primarily due to rapid, uncontrolled polymerization. This challenge arises because the absence of reversible bond formation between building blocks often leads to kinetically trapped, amorphous phases rather than the desired, thermodynamically stable crystalline structures. A significant advancement in COF synthesis has been achieved through the use of amphiphilic amino acid derivatives to form micelles, which act as templates for the formation of COF seeding crystals1. This innovative approach has successfully produced five single-crystal COF structures, enabling atomic-level structural elucidation. In this presentation, I will discuss the strategies employed to synthesize a range of 2D COFs using surfactant-based methods. I will also explore how this research was extended to the synthesis of novel 3D COFs, which are particularly difficult to achieve using traditional techniques. Additionally, I will provide a detailed analysis of the synthesized COFs, utilizing Powder X-Ray Diffraction and Scanning Electron Microscopy to confirm their crystal lattice structures. I will conclude by emphasizing how our research not only expands the structural diversity of COFs but also introduces a more eco-friendly and streamlined synthesis method compared to conventional approaches while paving the way for the fabrication of COF films with enhanced stability.

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Stimuli-responsive microcapsules for sustainable chemistry

Miss Hui Yang[1,2], Prof Jadranka Travas-Sejdic[1,2]
[1]The University of Auckland, Auckland, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand

Session 6C: Proteins and micelles, Dobson 2, February 11, 2025, 16:30 - 18:10

In recent decades, sustainable chemistry seeks to improve the efficiency with which natural resources are used to meet human needs for chemical products and services. Despite the progress made, waste generation incurs resource, time, and monetary costs during creation, handing, and end-of-life management. Especially, complex chemical transformations often required multiple steps, requiring separation, isolation, and purification resulting in material loss, higher energy consumption and time lost. Integrating these steps not only reduces waste but also lowers costs and enhances inherent safety. Nature is brilliant in its efficiently produce various chemicals and materials from local resources in ambient conditions, eliminating waste, and promoting life-friendly processes. That is, we should design the chemical synthesis processes to mimic natural systems. Artificial cell, imitating living cells, house various compartmentalized “organelles” enclosed by membranes, each serving specific physiological roles. The tight arrangement and dense packing of “organelles” enhance sequential enzymatic reactions, enabling effective bio-product transfer across compartments and reducing active intermediate degradation. In addition, hydrogels can serve as the membrane for artificial cell due to their responsiveness to stimuli such as swelling, shrinking, and degrading, enabling control over pore size and diffusion rates. Here, we aim to develop modifiable microcapsules made of hydrogels that can be tuneable via an external stimulus for use in cascade reactions. Through intricate design and precise control, these artificial cells made from hydrogel matrices can sensitively react to environmental cues, triggering dynamic changed in their behaviours. Such responsiveness allows artificial cells to act as miniaturized chemical factories and minimizing resource consumption.

Challenges in Connecting Casein Micelle Structure with Rheology of Skim Milk Concentrate

Mrs Cynthia Andriani[1,2], Dr Derek Knighton[3], Prof. Geoff Willmott[1,2], Associate Prof. Catherine Whitby[1,4], Prof. Bill William[3]
[1]MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand, [2]Departments of Physics and Chemistry, Faculty of Science, University of Auckland, Auckland, New Zealand, [3]Fonterra Research and Development Center, Palmerston North, New Zealand, [4]School of Food Technology and Natural Sciences, Massey University, Palmerston North, New Zealand

Session 6C: Proteins and micelles, Dobson 2, February 11, 2025, 16:30 - 18:10

As the main protein component in milk, casein plays a substantial role in the rheological properties of dairy-based products, including skim milk concentrate or SMC (1). However, understanding the rheology of SMC in connection with casein micelle structure in the nanoscale range can be challenging. In addition, this material is sensitive to shear rate, and the rheology varies significantly with its composition, temperature, and time. This study aims (a) to explore different structural analysis methods and (b) to connect the microstructural information with the viscosity at different temperatures T (55, 40, 20, 5 °C) and total solids TS (10 – 68 %w/w). SMC was prepared by vacuum-evaporating reconstituted skim milk powder, and bulk rheological measurements were done using a shear rate sweep (0.1–1000 s^{-1}). The structural investigation techniques tested on SMC samples include dynamic light scattering (DLS), environmental scanning electron microscopy (E-SEM), cryo-SEM, transmission electron microscopy (TEM), and cryo-TEM. The limitation of DLS is the necessity of working with a very dilute system. At the same time, the main limitation of the electron microscopy techniques is the preparation method that may alter the native structure of casein micelles in SMC. Further progress may be made using methods such as rheo-SAXS. Applying the Maron-Pierce-Quemada model (2, 3) to bulk rheology data found that the voluminosity decreases at high T and TS. This phenomenon can be related to deformation caused by the decreasing hydration capacity of casein micelles when TS > 40%, consistent with the cryo-SEM images.

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Bridging Scales: Advanced Simulations of Metal Hydride Materials for Hydrogen Storage

Dr Paul Jerabek[1], Prof Thomas Klassen[1,2], Dr Claudio Pistidda[1]
[1]Helmholtz-Zentrum Hereon, Institute of Hydrogen Technology, Geesthacht, Germany, [2]Helmut-Schmidt-University, Hamburg, Germany

Session 6D: Hydrogen storage materials, Dobson 3, February 11, 2025, 16:30 - 18:10

Metal hydride materials represent promising candidates for efficient, safe and long-term hydrogen storage due to their excellent volumetric storage densities that can promote a Greenhouse gas emission-free energy economy.

Our research group focuses on developing a multiscale simulation framework of interstitial room-temperature metal hydride materials (e.g. TiFe, LaNi5, CeNi5) to better understand and predict their physico-chemical properties and performance as stroage materials. By integrating quantum chemical calculations, molecular dynamics (MD), machine learning (ML), thermodynamics and mesoscale modeling, we bridge the gap between atomic-level interactions and macroscopic properties.

At the atomic scale, DFT calculations provide insight into the electronic structure to predict crystal structures of various phases, while (ab-initio) MD simulations capture the material responses under various conditions (temperatures, pressures) and help to shed light on the dynamic behavior of hydrogen atoms, such as diffusion pathways and kinetic barriers. [1] Moving to the mesoscale, we employ phase-field modeling based on our self-developed thermodynamic databases [2] [3] and calculated interfacial properties [4] to understand the evolution of microstructures during hydrogen absorption and desorption cycles.

This scale-bridging methodology not only accelerates material discovery but also offers valuable insights into the fundamental processes governing hydrogen-metal interactions. Our holistic approach enables us to predict material performance and will allow us to assess the role of additives and trace elements on hydrogen storage capacity, paving the way for sustainable materials development in-silico. [5]

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Assessing Impurity Effects on FeTi Alloys for Hydrogen Storage: A Multicomponent Thermodynamic Model

Ebert Alvares[1], Dr. Andrew J. E. Rowberg[2], Dr. Kai Sellschopp[1], Dr. Brandon C. Wood[1,2], Prof. Thomas Klassen[1,3], Dr. Paul Jerabek[1], Dr. -habil Claudio Pistidda[1]
[1]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany, [2]Quantum Simulation Group and Laboratory for Energy Applications for the Future (LEAF), Lawrence Livermore National Laboratory, Livermore, USA, [3]Helmut Schmidt University, Hamburg, Germany

Session 6D: Hydrogen storage materials, Dobson 3, February 11, 2025, 16:30 - 18:10

Hydrogen is a promising energy carrier as it can be produced through water electrolysis powered by renewable energy, and its combustion in fuel cell devices releases only water as a product. However, its efficient storage in gas or liquid form is energy inefficient due to the involved compression and cooling stages.

FeTi-based alloys offer an appealing solution to reversibly store large quantities of hydrogen compactly under near ambient operating temperature and pressure conditions. However, due to the sensitivity of the associated enthalpic properties to material composition, the hydrogenation properties of the resulting alloys may differ when FeTi is made from less pure raw and recycled materials. Understanding the effects of impurities is therefore crucial.

In this context, computational thermodynamic modeling is an essential tool for leveraging the production, design, and application of these materials. Yet, challenges arise when modeling multicomponent materials consisting of elements that have vastly different hydrogen affinities. To address this obstacle, this work presents a framework for modeling the thermodynamics of FeTi-based multicomponent hydrogen storage materials.

Based on thermodynamic analysis and first-principles calculations, the proposed model enables the description of hydrogenation properties under paraequilibrium — a specific state during the FeTi hydrogenation [1]. This work enhances the fundamental understanding of the composition-structure-properties relationships in multicomponent FeTi-based alloys for hydrogen storage, paving the way for advanced computational simulations of their hydrogenation.

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Exploring Hydrogen Storage in Silicon-Doped Ti-Fe Alloys Using Effective Bond Energy Formalism

Ms Lekshmi Dinachandran[1], Mr. Ebert Alvares[2], Dr. Kai Sellschopp[2], Dr. Paul Jerabek[2], Dr. Anna Garden[1]
[1]University Of Otago, Dunedin, New Zealand, [2]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon GmbH, Geesthacht, Germany

Session 6D: Hydrogen storage materials, Dobson 3, February 11, 2025, 16:30 - 18:10

The transition to a sustainable hydrogen economy is crucial for reducing the global reliance on finite fossil fuels and unstable non-conventional energy sources. A key aspect of this transition is ensuring safe and efficient hydrogen storage. Solid-state storage using metal hydrides like TiFe alloys offers significant advantages over gaseous or liquid hydrogen in terms of volume and energy efficiency. Aotearoa New Zealand's titanomagnetite ore deposits, rich in Ti and Fe intermetallic compounds, present a promising opportunity for hydride-based storage.

However, the presence of impurities in these ores raises critical questions: How do impurities affect hydrogen storage behavior, and how pure must TiFe be for optimal performance?

This study investigates the nanoscale processes in the hydrogenation and dehydrogenation of Si-doped TiFe alloys. Using Effective Bond Energy Formalism (EBEF) within a CALPHAD-based framework and supported by density functional theory (DFT), we model the effects of silicon and other impurities on the hydrogen storage capabilities of TiFe alloys. The EBEF approach simplifies computational complexity by breaking down the system into binary interactions, enabling the modeling of complex systems like the Laves phase in Si-doped TiFe.

This presentation will feature phase diagrams for TiFeSi and its hydrided form, calculated using EBEF/CALPHAD, and discuss the resulting thermodynamics of hydrogenation compared to pure TiFe. Understanding how impurities influence hydrogen storage will contribute to the broader goal of developing cost-effective, high-performance metal hydrides for hydrogen storage, potentially leveraging the benefits of natural impurities.

Nanometer-scale analysis of hydrogen storage in complex hydrides using small angle neutron scattering and simulations

Mr Arnab Majumdar[1], Prof. Martin Mueller[1,2,3], Dr. Sebastian Busch[1]
[1]GEMS at MLZ, Helmholtz Zentrum hereon, Garching b. Munich, Germany, [2]Institute of Material Physics, Helmholtz Zentrum hereon, Geesthacht, Germany, [3]IEAP, CAU Kiel, Kiel, Germany

Session 6D: Hydrogen storage materials, Dobson 3, February 11, 2025, 16:30 - 18:10

The current practice of using fossil fuels to satisfy the ever-growing energy demand is expected to cause an irreversible increase in temperature. Alternative fuels like hydrogen can be part of a solution to this problem due to its high gravimetric energy density. However, the low volumetric density of hydrogen in gas and liquid phases incurs problems related to storage [1]. To circumvent this problem, the chemical storage of hydrogen using a complex hydride system can be opted for. Amongst several options within complex hydrides, a mixture of $Mg(NH_2)_2$, $LiBH_4$, and LiH was chosen in this work to investigate using Small Angle Neutron Scattering (SANS) experiments and simulations [2].

SANS is commonly used to investigate nanoscale structures. In this work, in situ SANS measurements were performed to reveal information about the absorption and desorption of hydrogen on the nanometer length scale. However, the measurements do not allow a direct deduction of the process or structure in real space. Therefore, several models were proposed based on different hypotheses and the in situ SANS data was calculated from the simulation for comparison with experiments, accounting for all relevant instrument details [3,4,5].

As the simplest possible model, diffusion of hydrogen into and out of an isotropic grain of hydrogen storage material was hypothesized. The disparity between the simulation data and the experiment shows that a more complicated model is required to describe the experimental observation. Therefore, micro-structures of absorbed and desorbed states were generated probabilistically. The calculated data from the simulation is compatible with the experiments after adding micro-structural details.

Using the appropriate computational model and in situ SANS experiment, it was found that hydrogen gas must be partially entrapped on the nanometer length scale during desorption. Using the findings in the nanometer length scale, the volumetry performance related to the engineering length scale was predicted and a good match with the measurement was found.

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Synthesis of TiFe intermetallic for hydrogen storage applications via direct calciothermic reduction of ilmenite sand

Mr Zarar Rasheed[1], Dr. Chris Bumby[1], Dr Karl Dahm[2], Dr. Peng Cao[3], Dr. Claudio Pistidda[4]
[1]The MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, Wellington, New Zealand, [2]Callaghan Innovation, Wellington, New Zealand, [3]Faculty of Chemicals and Materials Engineering, University of Auckland, Auckland, New Zealand, [4]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Germany

Session 6D: Hydrogen storage materials, Dobson 3, February 11, 2025, 16:30 - 18:10

The transition to a hydrogen-based economy necessitates the exploration of safe, cost-effective energy carriers. The equiatomic intermetallic titanium-iron compound (TiFe) stands out as a promising solid-state hydrogen carrier due to its non-toxicity, high volumetric density, and safety attributes, particularly for stationary applications. However, the conventional synthesis of TiFe relies on titanium and iron as raw materials, posing environmental and economic challenges associated with titanium extraction. Here, we report experimental investigations into an alternative route to the production of TiFe through the direct reduction of ilmenite sand (FeTiO3), an abundant natural resource. The reduction process was conducted in a tube furnace under an argon atmosphere using calcium hydride (CaH2) as a reducing agent, and the impact of temperature and time has been systematically explored. Results indicate that a maximum TiFe yield of approximately 60 wt.% was achieved at 800 and 900°C for varying reduction times. For comparison, high-purity synthetic ilmenite was also reduced following the same approach, and this revealed a maximum TiFe yield of approximately 80 wt.%. Our findings confirm the potential for metallothermic direct-reduction of ilmenite sand as an economically viable alternative to the conventional TiFe production route.

Sustainable fabrication of MOF and Polyamide 12 composites for Advanced Hydrogen Storage through Selective Laser Sintering

Miss Chengming Shang[1], Dr Yaan Liu[1], Prof Oana Ghita[1], Dr Dong Wang[1], Prof Mi Tian[1]
[1]University Of Exeter, Exeter, United Kingdom

Session 6D: Hydrogen storage materials, Dobson 3, February 11, 2025, 16:30 - 18:10

Hydrogen storage is crucial for renewable energy advancement and a low-carbon economy, especially as a clean, efficient alternative to fossil fuels for transportation and energy storage. The challenge of designing next generation onboard hydrogen storage tank lies in storing hydrogen safely, compactly, and cost-effectively.

Metal-Organic Frameworks (MOFs) like MIL-101(Cr) are promising for hydrogen storage due to their high porosity and excellent gas adsorption properties[1, 2]. However, MOFs are often synthesized as polycrystalline powder, making them difficult to shape for industrial use. While Selective Laser Sintering (SLS) can create complex geometries and structures with high precision.

This research aims in the development of tank systems based on the fabricating MOF-polymer composites tank-filler to enhance hydrogen storage performance using an innovative method: slow-drying. To fully understand this new method, the effectiveness of each experimental parameter was investigated through 19 experiments using fractional factorial design methodology. Our results demonstrated the optimized parameters for achieving the best hydrogen storage performance in this novel MOF-polymer composites fabrication method. These findings open new avenues for shaping MOFs and improving the compatibility of MOF-polymer applications in next generation hydrogen storage tank system and related fields, including onboard hydrogen storage, offering possibilities for designing other MOF-polymer composites.

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The role of ergodicity in the performance of memristive reservoir computing

Dr Valentina Baccetti[1], Dr Ruomin Zhu[2,3], Professor Zdenka Kuncic[3], Dr Francesco Caravelli[4]
[1]Rmit University, Melbourne, Australia, [2]McMahon Lab Cornell University, Ithaca, USA, [3]University of Sydney, Sydney, Australia, [4]Los Alamos National Laboratory, Los Alamos, USA

Session 6E: Neuromorphic unconventional and physical computing Symposium, Dobson 4,
February 11, 2025, 16:30 - 18:00

Networks composed of nanoscale memristive components, such as nanowire and nanoparticle networks, have recently received considerable attention because of their potential use as physical reservoir computing systems [1,2].

A significant characteristic of nanoscale memristive network is the presence of various conductance transitions of first and second order. These transitions, which often involve transiently unstable dynamics of the memristive components, have been interpreted as critical “dynamical” states —sometimes referred to as the "edge of chaos"—and are believed to be important for the performance of reservoir computing [3].

Scope of this talk is to demonstrate how the network’s ergodicity level can be considered a relevant predictor of conductance/resistance transitions. This is because the concept of ergodicity implies that a system’s long-term dynamic evolution can be predicted using short-term observations. Furthermore, in memory-dependent systems (such as in memristive networks), lack of ergodic behaviour is associated with symmetry breaking and phase transitions [4].

We begin by confirming that the performance on machine learning tasks improves when a reservoir composed of ideal memristors [5] is tuned to operate close to a conductance transition point.

We then use the Thirumalai-Mountain fluctuating metric [6], a quantitative measure of ergodicity breaking levels, to show that this optimal operational regime corresponds to non-ergodic dynamics of the memristive reservoir.

These results highlight a potential strong connection between emergence of memory, symmetry breaking dynamical transition - indicated by non-ergodic dynamics - and reservoir’s learning performance [7].

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Research Software and Machine Learning Practices in Neuromorphic Computing: A Comprehensive Analysis and Roadmap

Mr Ryan Daniels[1]
[1]Accelerate Programme for Scientific Discovery, Department of Computer Science and Technology, University of Cambridge, Cambridge, United Kingdom

Session 6E: Neuromorphic unconventional and physical computing Symposium, Dobson 4,
February 11, 2025, 16:30 - 18:00

Neuromorphic computing has emerged as a promising paradigm for unconventional computing systems within materials science. From simulations to data analysis, software has become indispensable in advancing this field. However, the reproducibility of results remains a challenge, highlighting the critical need for open scrutiny of research software [1].

This submission presents a comprehensive review of neuromorphic computing literature from a leading journal. We systematically evaluate publications using criteria and methods adapted from established journals and conferences [2-4], focusing on software-related aspects such as open-source availability, licensing, testing protocols, reproducibility steps, and documentation quality.

Our findings reveal concerning trends in the reproducibility of neuromorphic computing research. In papers performing computational tasks, less than half compare their results to established baselines, and only one third discuss crucial machine learning elements like hyperparameter optimization and data splits. Alarmingly, only one quarter of papers released any code, and among those with available code, significant issues persist in licensing, testing, and documentation.

Based on these insights, we propose a roadmap for enhancing reproducibility in neuromorphic computing research, emphasizing the need for transparent software practices. This includes recommendations for open-source code sharing, standardized documentation, and comprehensive testing. Adopting these practices is crucial for accelerating progress and ensuring the reliability of reported advancements in this software-driven field. By highlighting the current state of reproducibility and offering concrete steps, this work aims to foster a more robust and transparent research ecosystem in the rapidly evolving domain of neuromorphic computing and materials science at large.

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Dynamics of induced pathways in thermistor grid networks

A/Prof Matthew Arnold[1], Mr Angelo Vitaliti[1], Prof Simon Brown[2]
[1]University Of Technology Sydney, Sydney, Australia, [2]University of Canterbury, Christchurch, New Zealand

Session 6E: Neuromorphic unconventional and physical computing Symposium, Dobson 4, February 11, 2025, 16:30 - 18:00

In-materio simulation of differential equations has potential for efficient solution of network transport problems[1]. Optimization of networks requires an ability to rapidly configure and test a large number of different possibilities[2]. Thermistor grid networks offer a simple physical model of dynamic transport networks that can be reconfigured with local thermal sources. Here, as a first step towards using these networks for transport calculation, we simulate the stability of induced thermal patterns under external electrical and thermal bias. Starting from the multistable states of a single thermistor we establish feasible bounds for steady-state conduction in grid networks. We then examine the stability of progressively more complicated paths, starting from single straight lines to zig-zag paths of differing amplitudes and periods.

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Fabrication and characterization of S- shaped dinaphthothienothiophene (S-DNTT) OFETs based on silicon substrates

Mr. Rafael Ashkrizzadeh[1], Mrs. Lynn Schwäke[2], Mr. Moritz Peitzner[1], Mr. Adrian Petraru[1], Mr. Franz Faupel[2], Mr. Hermann Kohlstedt[1], Mr. Stefan Schröder[2]
[1]Chair of Nanoelectronics, Faculty of engeneering, Kiel university, Kiel, Germany, [2]Chair for Multicomponent Materials, Faculty of engeneering, Kiel university, Kiel, Germany

Session 6E: Neuromorphic unconventional and physical computing Symposium, Dobson 4,
February 11, 2025, 16:30 - 18:00

Organic field effect transistors (OFETs) have been attracting great interest due to their use on flexible substrates. The use of organic small molecular semiconductors allows for processing on different substrates through low-cost fabrication techniques such as spin coating and drop-casting. Established organic semiconductors like rubrene and pentacene are well known but typically prone to oxidation in ambient conditions and only a limited solubility. This work discusses the fabrication and characteristics of OFETs using S-DNTT 10 [1] as the semiconductor material. S-DNTT 10 is highlighted for its advantageous properties, including good solubility and enhanced stability in ambient conditions. These properties make S-DNTT 10 particularly suitable for the low-cost fabrication of OFETs in ambient conditions.

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Thickness dependent (analog) switching in SiOx/Cu/SiOx memristive devices

Mr Rouven Lamprecht[1], Mr Tobias Gergs[2], Mrs Sahitya Yarragolla[2], Mr Ole Gronenberg[3], Mr Richard Marquardt[1], Mr Finn Zahari[1], Mr Jan Trieschmann[2], Mr Hermann Kohlstedt[1]
[1]Chair of Nanoelectronics, University of Kiel, Kiel, Germany, [2]Theoretical Electrical Engineering, University of Kiel, Kiel, Germany, [3]Synthesis and Real Structure Group, University of Kiel, Kiel, Germany

Session 6E: Neuromorphic unconventional and physical computing Symposium, Dobson 4,
February 11, 2025, 16:30 - 18:00

Memristive devices for neuromorphic circuits represent an emerging nanotechnology with significant potential for bio-inspired computing architectures. With their characteristic voltage-dependent resistance, the functionality of these devices may be considered analogous to synapses in biological nervous systems. Like their biological counterparts, it is crucial to adapt their properties for specific tasks. In this work, we integrate experimental and modeling techniques to systematically analyze the electrical properties of memristive devices, targeting a knowledge-driven design. The devices were fabricated using various processing techniques (i.e., thermal evaporation and magnetron sputtering) subject to respectively different parameters. Our experimental data includes localized measurements of current-voltage (I-V) characteristics, showcasing the analog switching behavior of TiN/SiOx/Cu/SiOx/TiN memristive devices. This is complemented by a structural analysis of the device stack. Monte Carlo simulations further elucidate the impact of fabrication conditions by modeling both the deposition sources and the composition of the resulting thin films. Through this study, we establish correlations between the observed electrical properties of the devices and the simulated deposition parameters, offering valuable insights into the critical operational conditions that affect analog memristive behavior.

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A Catalyst Life and its Circumstances

Professor Beatriz Roldan Cuenya[1]
[1]Fritz-haber-Institute of Max Planck Society, Berlin, Germany

Plenary Session 4, Auditorium, February 12, 2025, 08:30 - 09:30

Climate change concerns have spurred a growing interest in developing environmentally friendly technologies for green energy generation and storage in the form of chemical bonds. The latter includes green H2 production from water splitting and the re-utilization of CO2 via its thermal or electrocatalytic reduction into value-added chemicals and fuels. Moreover, alternative methods for ammonia synthesis either with green H2 or direct electrocatalytic NH3 synthesis are also being sought in order to reduce carbon emissions, while providing a transport energy carrier for green hydrogen. In this context, it is thus important to develop low cost, highly efficient and durable catalysts with tunable selectivity. This requires understanding the evolution of their structure and surface/bulk composition under reaction conditions, i.e. while the active sites are formed or become poisoned leading to their deactivation.

This talk will offer new mechanistic insights into the electrocatalytic reduction of CO2 and nitrate reduction as well as the oxygen evolution reaction using model pre-catalysts ranging from single atoms, size- and shape-controlled nanoparticles, epitaxial thin films to single crystals. I will illustrate the need of a multi-technique operando microscopy and spectroscopy approach, when possible combined, to gain understanding into the complex evolution of electrocatalytic materials while at work. Examples will be given on the correlation between their dynamically evolving structure and composition and their activity and selectivity.

These results are expected to open up new routes for the reutilization of CO2 through its direct conversion into industrially valuable chemicals and fuels such as ethylene, methanol and ethanol, and the generation of green H2 and ammonia via electrolysis.

Perovskite Quantum Dots for Solar Cells and Beyond

Professor Lianzhou Wang[1]
[1]The University of Queensland, Brisbane, Australia

Keynote Session 10, Auditorium, February 12, 2025, 09:35 - 10:10

Halide perovskite solar cells have witnessed great successes recently while their instability is a big hurdle for practical application. Herein we discuss our recent progress in addressing the stability of perovskite solar cells, including introduction of capping layers to improve the stability against moisture and heat, and perovskite size engineering to suppress phase segregation. In particular, quantum dots (QDs) have the advantages of quantum confinement effect, defect-tolerant nature, and processability for flexible devices. We discuss a new colloidal surface ligand engineering strategy in designing new hybrid perovskite QDs with controllable compositions and sizes The QDs have been used as building blocks in quantum dot solar cells delivering a certified record efficiency of 16.6% with excellent long-term operation stability. By using QDs as light absorbing materials, the QD based photocatalysts also exhibited good stable performance in photocatalytic hydrogen production. The combination of perovskite QDs with Metal-Organic Framework (MOF) materials to form new composites led to ultrastable photoluminescent property for > 10,000 hours. The integration of perovskite solar cells and rechargeable batteries have led to a single module type rechargeable solar batteries with an overall storable solar energy conversion efficiency of >12%.

Multilayer spintronic neural networks with radio-frequency connections

Dr Frank Mizrahi[1]
[1]Laboratoire Albert Fert, Palaiseau, France

Keynote Session 11, Dobson 4, February 12, 2025, 09:35 - 10:10

Spintronic nano-synapses and nano-neurons perform neural network operations with high accuracy thanks to their rich, reproducible and controllable magnetization dynamics. These dynamical nanodevices could transform artificial intelligence hardware, provided that they implement state-of-the art deep neural networks. However, there is today no scalable way to connect them in multilayers.

Here we show that the flagship nano-components of spintronics, magnetic tunnel junctions, can be connected into multilayer neural networks where they implement both synapses and neurons thanks to their magnetization dynamics, and communicate by processing, transmitting and receiving radio frequency (RF) signals.

We build a hardware spintronic neural network composed of nine magnetic tunnel junctions connected in two layers, and show that it natively classifies nonlinearly-separable RF inputs with an accuracy of 97.7%.

Using physical simulations, we demonstrate that a large network of nanoscale junctions can achieve state-of the-art identification of drones from their RF transmissions, without digitization, and consuming only a few milliwatts, which constitutes a gain of several orders of magnitude in power consumption compared to currently used techniques.

This study lays the foundation for deep, dynamical, spintronic neural networks [1].

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Highly tuneable hydrogen evolution catalysts of MoS2 on 2D carbon-based supports

A/Prof Anna Garden[1], Charlie Ruffman, Chris Mills, Kayla Prendergast, James Gilmour
[1]University of Otago, Dunedin, New Zealand

Session 7A: Computational materials and modelling, Auditorium, February 12, 2025, 10:40 - 12:40

Hydrogen (H_2) is becoming increasingly established as a promising alternative to traditional fossil fuels, yet it relies on a cheap and clean method of production. The electrocatalytic hydrogen evolution reaction (HER) is one of the leading technologies for cheap and clean H_2 production. Platinum (Pt) is one of the most effective HER catalysts but its scarcity and associated cost prohibits widespread use and cheaper, Earth-abundant catalysts are sought. Nanoscale MoS_2 catalysts have been identified as promising catalysts, showing modest HER activity. However, the activity still falls short of that of Pt and further optimisation to the catalyst is required for it to be competitive with Pt.

This presentation will explore recent results from detailed density functional theory (DFT) calculations of the HER activity on MoS_2 catalysts supported by a range of 2D carbon-based supports. We find that the activity is highly tuneable and the reasons for the tunability are elucidated for a range of MoS_2 morphologies and active sites.

Rational Catalyst Design for CO2 Electrochemical Reduction Reaction

Ziyun Wang[1]
[1]The University of Auckland, Auckland, New Zealand

Session 7A: Computational materials and modelling, Auditorium, February 12, 2025, 10:40 - 12:40

Electrochemical CO2 reduction (CO2RR) offers a promising route for converting CO2 into valuable chemicals and fuels using renewable electricity [1]. However, significant challenges remain in terms of product selectivity, energy efficiency, and long-term stability, particularly when using industrially-relevant CO2 sources. This talk will present recent advancements in CO2RR, drawing from several cutting-edge studies that address these challenges from multiple angles.

In this talk, we will first introduce a general computational framework for catalyst design [2]. Then, we will use density functional theory (DFT) calculations to understand the reaction pathways of CO2RR to multiple products. The reaction barriers and enthalpy changes are calculated for the elementary steps considered in all the pathways on Cu(100). We will then introduce the selectivity determinants based on microkinetic modelling.

Furthermore, we will discuss novel catalyst designs, including cationic-group-functionalized copper catalysts that enable stable acidic CO2 electrolysis with high selectivity towards multi-carbon products [3]. The role of the catalyst-electrolyte interface in promoting CO2 activation while suppressing competing reactions will be examined. We'll also explore system-level innovations, such as proton-exchange membrane electrolysers that achieve durable CO2 conversion to formic acid using recycled lead catalysts [4].

Furthermore, we'll address the critical issue of catalyst poisoning by trace impurities in industrial CO2 streams, presenting strategies to improve SO2 tolerance through rational catalyst and electrode design[5]. By integrating insights from catalyst development, reaction mechanisms, and electrolyser engineering, this work demonstrates significant progress towards making CO2 electrolysis a viable technology for large-scale carbon utilization and renewable fuel production.

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Computational materials discovery for new battery electrode materials

Dr Joseph Nelson[1]
[1]Lincoln Agritech, Christchurch, New Zealand

Session 7A: Computational materials and modelling, Auditorium, February 12, 2025, 10:40 - 12:40

Rechargeable batteries power modern society, and are found in devices ranging from mobile phones and laptops to electric vehicles. Large-scale batteries are also expected to play a key role in future renewable energy networks, to smooth out fluctuations in energy supply.

In this presentation, we focus on the Li and Na-ion class of batteries and discuss how computational materials discovery can be leveraged to find new and improved battery electrode materials [1]. Such materials are a key step in producing batteries with higher capacities, improved cyclabilities, or reduced environmental impact.

Our computational discovery process uses density-functional theory (DFT) calculations in conjunction with the ab initio random structure search (AIRSS) technique for generating candidate material structures [2,3]. These techniques allow in-depth insight into nanoscale-level changes that occur in electrodes upon battery charge and discharge. We highlight some recent success stories with this approach, particularly in the Na-ion space [4,5].

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Implementing Machine Learning Towards Nanocluster Global Optimisation

Mr Elouan Hay-Fourmond[1], Associate Professor Anna Garden[1]
[1]University of Otago, Dunedin, New Zealand

Session 7A: Computational materials and modelling, Auditorium, February 12, 2025, 10:40 - 12:40

Nanoclusters are polyatomic aggregates with unique properties heavily influenced by their structure that lie between those of bulk materials and individual atoms. Some of these exhibit catalytic capabilities such as CO2 reduction. However, due to the multitude of possible conformers for each cluster, finding the most stable, or lowest energy structure (global minimum), is a computational challenge. While global optimisation methods have greatly minimised this challenge, the process can still be incredibly expensive as it might still require thousands of local optimisations. We aim to further reduce the costs of this process by implementing machine learning.

In this project, machine learning will be used with the aim of speeding up each individual optimisation task. An active learning approach will be used such that training the machine learning algorithm and running the optimisation are completed at the same time. The Vienna Ab Initio Simulation Package (VASP) machine learning implementation and density functional theory (DFT) will be used for this project. Various parameters and approaches will be evaluated to assess the potential speed increases and the quality of the model's predictions for energies and forces. The approach will be applied to Cu, Au, and Pt nanoclusters of varying sizes. This could significantly lower computational costs, making cluster global optimisation more accessible.

Developing machine learning models for atomistic simulations: Potential applications and prospects in metal hydride materials

Ms Archa Santhosh[1], Dr Kai Sellshopp[1], Prof Thomas Klassen[1,2], Dr Paul Jerabek[1], Prof Claudio Pistidda[1]
[1]Helmholtz-zentrum Hereon, Max-Planck-Straße 1, D-21502 Geesthacht, Germany, [2]Helmut-Schmidt-Universität - Universität der Bundeswehr, Holstenhofweg 85, 22043 Hamburg, Germany

Session 7A: Computational materials and modelling, Auditorium, February 12, 2025, 10:40 - 12:40

Machine learning (ML) methods in computational material science offer immense potential in material design, discovery and engineering. In large-scale molecuar dynamics (MD), well trained ML interatomic models provide a much-desired balance between speed and chemical accuracy. In this work, this is demonstrated with succesfully trained deep neural network models (DNN) for two prominent metal hydride systems, TiFe and LaNi5. The DNN models for Ti-Fe-H and La-Ni-H systems are trained and validated with ab-initio molecular dynamics (AIMD) data. In performance, they far exceed the time and length-scales accessible with pure ab-initio methodology accomplishing 1000 times the speed of AIMD while retaining quantum chemical accuracy.

The Ti-Fe-H DNN model is utilized for exploring the dynamics of hydrogen interactions in the material lattice and performs very well for most common unary, binary and ternary phases in the Ti-Fe-H system. The DNN model for La-Ni-H system was built specifically for assessing the radiation tolerance of LaNi5 and its hydride phases for their potential hydrogen storage applications in cosmic environments. This model is used to understand defect generation and their evolution dynamics in relevant La-Ni-H phases, which in essence is unachievable with most ab-initio approaches. The accuracy necessary here also makes the use of empirical or semi-empirical potentials infeasible. These ML model thus provide a prime example as an ideal bridging tool for atomistic simulations.

Furthermore, future prospects and potential diverse applications for ML methods with a focus on emerging materials like compositionally complex alloys are also explored.

Halogen Bonding within Ionic Liquids

Dr Muhammad Ali Hashmi[1], Prof. Patricia Hunt
[1]Victoria University Of Wellington, Wellington, New Zealand

Session 7A: Computational materials and modelling, Auditorium, February 12, 2025, 10:40 - 12:40

Ionic liquids (ILs) have gained significant attention in chemical and industrial applications due to their versatile roles as electrolytes, green solvents, and catalysts. ILs deliver a unique combination of properties, including low vapour pressure, nonflammability, high thermal conductivity and stability, a broad electrochemical window, and customisable solvation ability. Hydrogen bonding (H-bonding) in ILs has been explored and contributes to IL physico-chemical properties.1 Halogen bonding (X-bonding) is emerging as a versatile bonding mode within a variety of fields, including materials chemistry, crystal engineering, anion sensing and organocatalysis.2 The concept of X-bonding in ILs is a novel area of research. ILs can be functionalised with X=Br or I atoms, leading to the polarisation of the electron density in the C-X σ-bond and the creation of an electron-deficient area (σ-hole) at the outmost portion of the halogen along the axis of the C-X bond. The σ-hole (δ+) and anion (δ-) can form an attraction called the X-bond. In this study, X-bonding interactions have been investigated for a range of imidazolium and ammonium-based ILs. Ion pairs (IPs), including 1-ethyl-3-methyl-imidazolium chloride, have been optimised, and the σ-holes characterised. The effect of the anion on the σ-hole and in forming an X-bond has been examined. The structure of the cations has been modified to control the magnitude of the σ-hole, with the aim of developing rational design principles for X-bonding interactions within ILs.

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Singlet Fission Enhanced 2d Perovskite Solar Cells

Dr Nate Davis[1]
[1]Victoria University of Wellington, Wellington, New Zealand

Session 7B: Photovoltaics and light harvesting, Dobson 1, February 12, 2025, 10:40 - 12:40

Most photovoltaics (PVs) exhibit a single absorption threshold, which means any excess energy is wasted and the maximum efficiency a PV can achieve is ≈ 32%. The main loss mechanism responsible for this low efficiency is thermalisation. We have fabricated and patented a new hybrid material that consists of two components, an organic interlayer of molecules which can undergo singlet fission (SF) (an excitation multiplication process) sandwiched between 2D-layers of perovskite semiconductor material. The SF material transfers its multiple excitations to the perovskite material resulting in two excitations per high-energy photon received. Focusing on emerging solution processable PV technologies, such as perovskites, offers more desirable and ambitious outcomes such as cost and manufacturing simplicity.

Exceeding 2.2 V Open-Circuit Voltage in Perovskite/Organic Tandem Solar Cells via Multi-Functional Hole-Selective Layer

Mr. Jung Geon Son[1], Dr. Shahid Ameen[1], Professor BongSoo Kim[1], Professor Dong Suk Kim[1], Professor Jin Young Kim[1]
[1]Ulsan National Institute of Science and Technology (UNIST), Ulsan, South Korea

Session 7B: Photovoltaics and light harvesting, Dobson 1, February 12, 2025, 10:40 - 12:40

Perovskite/organic tandem solar cells (POTSCs) are gaining attention due to their potential to surpass the Shockley-Queisser limit through the reduction of thermalization losses. However, wide bandgap perovskite solar cells (WBG PSCs), which function as top cells of POTSCs, still suffer from significant open-circuit voltage (VOC) loss, which limits the efficiency improvement of POTSCs. Here, we report a multi-functional hole-selective layer (mHSL) via blending two functionalized molecules (4-(3,6-diiodo-9H-carbazol-9-yl)butyl)phosphonic acid (36ICzC4PA) and (4-(3,6-dimethoxy-9H-carbazol-9-yl)butyl)phosphonic acid (36MeOCzC4PA). The blending of the two highly aggregating molecules demicellizes to form a uniform and high-coverage mHSL, which plays multiple roles of (i) providing the homogeneous surface potential of the HSL, (ii) extracting hole efficiently, (iii) enhancing the crystallinity of the perovskite on mHSL, and (iv) suppressing both lattice strain and phase segregation. Thus, it maximizes the VOC in POTSCs. Implementing mHSL on WBG PSCs enables a power conversion efficiency (PCE) of 18.85% with a notable VOC of 1.366 V. When applied to fabricated POTSCs, the PCE reached 24.73% (certified 24.19%) with a record-high VOC and fill factor (FF) of 2.216 V and 84.07%, respectively. Furthermore, encapsulated POTSCs exhibit excellent photostability, retaining 80% of their initial PCEs after maximum power point (MPP) tracking under 1-sun illumination in ambient conditions for 305 hours. In addition, unencapsulated POTSCs demonstrate notable thermal stability, retaining 82% of their initial PCEs after exposure to 65℃ in N2 conditions for 500 hours.

Symmetry Breaking Charge Separation in Linked Violanthrone Dimers

Dr Nina I. Novikova[1], Dr. Mina Barzegaramirolia[1], Dr. Wallace W. H. Wong[1], Prof. Ken P. Ghiggino[1]
[1]The University of Melbourne, Melbourne, Australia

Session 7B: Photovoltaics and light harvesting, Dobson 1, February 12, 2025, 10:40 - 12:40

Charge separation is a fundamental process in photophysical and photochemical systems, crucial for the conversion of light energy into chemical energy. Natural systems have perfected energy harvesting and charge separation and are a source of inspiration when developing efficient photonic materials. Symmetry breaking charge transfer in the 'special pair' of photosynthetic systems is one such example.

Herein I will focus on violanthrone dimers as novel chromophores exhibiting symmetry breaking charge transfer. Violanthrone derivatives have been suggested for applications in light upconversion and singlet fission due to favourable energetics and chemical stability.[1] Some violanthrones have triplet state energies below excited oxygen and have proved useful components in upconverting solar radiation below the silicon bandgap. Intermolecular interactions between violanthrone electronic states are an important factor in determining the efficiency of these photo-induced processes. In this work we have investigated the photophysics of several novel covalently linked violanthrone dimers using ultrafast laser spectroscopy. Photoexcitation of violanthone dimers in polar solvents leads to strong fluorescence quenching compared to non-polar solvents, with transient spectra exhibiting a new absorption band and spectro-electrochemistry confirming this new band as a reduced species of violanthrone. The rate of charge separation is sensitive to the orientation and distance between the two chromophores relative to each other and can be tuned by modification to the covalent linkage between the two dimer components. If time permits, I will introduce our exploration of the effect of linkers on charge separation and recombination in porphyrin-NDI donor-acceptor systems.

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Morphology control of Y6 thin films in single-component solar cells

Mr Nikita Shumilov[1,2], Ms Aditi Kumar[1,2], Dr Nathaniel Davis[1,2], Dr Michael Price[3], Dr Paul Hume[1,2], Professor Justin Hodgkiss[1,2]
[1]Victoria University of Wellington, Wellington, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand, [3]University of Bristol, Bristol, United Kingdom

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Organic photovoltaics (OPVs) is a rapidly growing and promising field in science and technology. Devices based on organic compounds offer advantages like flexibility, biocompatibility, and cost-effective manufacturing. However, the low dielectric constants in organic semiconductors necessitate the presence of a molecular heterojunction to split excitons into charges, limiting the OPV performance. Recently, non-fullerene acceptors (NFAs) with relatively high dielectric constants have shown the ability to generate charges without the need for a heterojunction.1 Despite this advancement, problems like charge traps and recombination still hinder the efficiencies of single-component OPV devices. Optimising the morphology of non-fullerene acceptors (NFAs) like Y6 is still underexplored in organic electronics. Understanding how different Y6 morphologies impact its optoelectronic properties, such as charge generation and charge-transfer states, is key to developing highly efficient hetero/homo-junction devices. In this study, we focused on the device aspect of the research and prepared Y6-based single-component solar cells with “as-cast”, “co-facial”, and “end-on” molecular orientations. The results indicate that the device absorption spectra for the “co-facial”, “as-cast”, and “end-on” films have the lowest to highest intensities in that order. However, the quantum efficiency measurements reveal that the “as-cast” based devices have the highest photon to exciton conversion efficiency. Nevertheless, while devices based on "co-facial" and "end-on" films achieve efficiencies of only 0.0013% and 0.0086%, respectively, the "as-cast" film integrates the most advantageous features of both morphologies, resulting in the highest OPV device efficiency of 0.0165% among the studied morphologies.

Magneto- versus Electro- caloric effects and what they can tell us

Professor Annie Powell[1]
[1]Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

7C: Spintronics and magnetic effects, Dobson 2, February 12, 2025, 10:40 - 12:40

A fascination for us all is understanding the interplay of electric and magnetic components of electromagnetic radiation in shaping the Universe. Although we concentrate on the "visible" nature of this radiation, we also know that most of the Universe is invisible and exists in the form of dark matter and energy. In addition, although we understand well how electric fields can be modelled in terms of the electrically polarised properties of electrons, we still do not really grasp the concept of spin nor the missing aspect of a polarised spin of electrons in terms of a magnon. This has consequences on the interpretation of electro- and magneto-caloric effects. Both demand an adiabatic component which is steered by a polarised electromagnetic field and much easier to realise for magnetic rather than electric components. On the other hand, we recognise that the electric part of an electromagnetic field is a dipole whereas the magnetic part is a monopole (here the idea of a magnon).

I will present some examples to elucidate this with a particular emphasis on molecules where a magnetically dark state can be realised and thus contribute to our understanding of dark matter and energy.

There will be a particular emphasis on using Maxwell's equations, better described as Maxwell-Heaviside [1] equations, to gauge the contributions of electronic and magnetic components to caloric effects.

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Forming ultimately tunable magnetic materials; fundamental interests in spin-orbit physics to applications in cryogenic electronics

Dr William Holmes-hewett[1,2], Dr. Jackson Miller[1,2], Catherine Pot[2,3], Dr. Simon Granville[1,2], Dr. Bob Buckley[1,2], Dr. Joe Trodahl[3], Dr. Ben Ruck[2,3]
[1]Robinson Research Institute, Victoria University Of Wellington, Wellington, New Zealand, [2]The MacDiarmid Institute for Advanced Materials and Nanotechnology, , New Zealand, [3]School of Chemical and Physical Sciences, Victoria University Of Wellington, Wellington, New Zealand

7C: Spintronics and magnetic effects, Dobson 2, February 12, 2025, 10:40 - 12:40

At the cryogenic temperatures required for the operation of next generation superconducting and quantum computing systems conventional memory systems do not operate. For the promised advances of these technologies to be realised a viable cryogenic memory must be developed. Designs for these systems exist, but the materials to realise these designs do not.

Here we present our work forming versatile magnetic materials from various rare-earth nitrides. These materials are dopable semiconductors with a conductivity tunable over orders of magnitude, most have a ferromagnetic ground state at cryogenic temperatures. The combination and competition of spin and un-quenched orbital angular momentum on the tri-valent rare-earth ions further allows the tuning of various magnetic properties. Using combinations of lanthanide ions in the nitride we demonstrate independent control of the net-magnetisation, coercive and exchange fields. We will describe the application of these materials in a cryogenic memory device for integration with existing superconducting logic and the advantages and exploration of novel magnetic Josephson junctions containing these materials.

Efficient generation, conversion and manipulation of electron and photon spins in semiconductor nanostructures for room-temperature opto-spintronics

Y Huang[1], V Polojärvi[2], S Hiura[3], P Höjer[1], A Aho[2], R Isoaho[2], T Hakkarainen[2], M Guina[2], S Sato[3], J Takayama[3], A Murayama[3], I.A Buyanova[1], Professor Weimin Chen[1]
[1]Linköping University, Linköping, Sweden, [2]Tampere University, Finland, [3]Hokkaido University, Japan

7C: Spintronics and magnetic effects, Dobson 2, February 12, 2025, 10:40 - 12:40

Semiconductor spintronics holds the potential for opto-spintronics that will allow integration of spin-based information processing and storage with photon-based information transfer. Unfortunately, progresses of semiconductor spintronics have so far been severely hampered by the failure to generate nearly fully spin-polarized charge carriers at and above room temperature (RT). In this work, by exploring a new approach of defect-engineered remote spin filtering, we succeeded in achieving conduction electron spin polarization exceeding 90% at RT in InAs/GaAs quantum-dots (QDs) [1] - the highest RT electron spin polarization ever reported in any semiconductor by any approach! The achieved electron spin polarization can be one-to-one converted to optical polarization of the QD light emissions. We also uncover spin nonlinearity in such opto-spintronic nanostructures, which enables harmonic generations of spin modulation at a frequency potentially approaching THz [2]. We further show that the QD electron spin can be remotely manipulated by spin control in the adjacent GaNAs spin filter, providing an opportunity for remote spin encoding and writing of quantum memory as well as for remote spin control of spin-photon interfaces. This work demonstrates the feasibility to implement opto-spintronic functionality under practical device operation conditions in a semiconductor nanostructure system based on the mature III-V semiconductor technology commonly used for today's optoelectronics and photonics. It could also pave the way for a range of potential spintronic and opto-spintronic applications exploiting the state-of-the-art GaAs technology platform, such as spin-LEDs, spin lasers, spin-polarized single-photon sources, quantum spin-photon interfaces, spin qubits.

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Spin-selective electron transfer in chiral materials: Towards the next generation of spintronics

Dr Muhammad Hanif[1,2], Joshua S. Webb[1,2], Wei-Hsiang Liao[3], Dr Simon Granville[2,4], Professor Hua-Shu Hsu[3]
[1]School of Chemical Sciences, The University of Auckland, Auckland, New Zealand, [2]The MacDiarmid Institute for Advanced Materials and Nanotechnology, New Zealand, [3]Department of Applied Physics, National Pingtung University, Pingtung, Taiwan, [4]Robinson Research Institute, Victoria University of Wellington, Wellington, New Zealand

7C: Spintronics and magnetic effects, Dobson 2, February 12, 2025, 10:40 - 12:40

Chirality plays a critical role in a plethora of phenomena, from physics to chemistry to medicines. Recent studies have shown that chirality in molecules and materials offers a new way of controlling and manipulating electron spin. [1-4] When electrons pass through chiral molecules, one spin orientation is preferred over the other. This chirality-induced spin selectivity (CISS) [2,3] means that electron transmission through chiral materials is spin-selective, producing a spin-polarised current. This property is important since spin currents generated from chiral structures do not dissipate energy through resistive heating.[5] Moreover, CISS and spin-polarised currents will enable spin-dependent photoluminescence,[6] spin light-emitting diodes,[1] enantiospecific electrochemistry,[7] spin-selective electrocatalysis,[8,9] and new quantum devices and quantum information processing methods.[2,10]

We have prepared chiral metallopolymers that combine the chirality of biomolecules, such as amino acids, with the conducting properties of metal ions. These metallopolymers are highly tuneable, through a systematic variation of metal ions and chiral ligands, to optimise key factors such as conductivity, spin-orbit coupling, and magnetic moment/exchange interactions.[11,12] In this talk, I will discuss the synthesis of chiral coordination polymers, as well as their spin polarization and spin-selective properties.

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Small but Mighty? Innovation, Policy and Sustainability Transitions in New Zealand and its OECD Peers

Professor Kira Matus[1], Dr. Viktoria Doeme
[1]The Hong Kong University of Science and Technology, Clearwater Bay, Hong Kong

Session 7D: Science commercialisation, Dobson 3, February 12, 2025, 10:40 - 12:40

What is the role of government policy in supporting an innovation system that successfully links academia and industry? Innovation plays an inevitable role in transforming societies towards sustainable development. While this has been well acknowledged by policymakers, it remains unclear what policy approaches governments have taken to impact the underlying innovation strategies and policies. Furthermore, although there is extensive academic literature suggesting how innovation policy should deal with sustainability transitions, it largely relies on in-depth case and small-n studies with a focus on a limited number of sectors and, especially large, countries. Yet many of the leading nations in terms of both sustainability and technological innovation are small, high-income countries with populations of 4-10 million.

To better understand the government strategies that underly the relative success of these small nations, which includes New Zealand, we provide a comprehensive multi-sectoral (agriculture, water, health, energy, and manufacturing) and multi-country (10 smaller developed and innovative countries) analysis, examining a novel dataset of 1722 sustainability-related policy interventions from 2008-2020. This presentation will focus on our findings specific to New Zealand in the context of its peers, including identifying key policies, public sector actors, and gaps in its policy approach. We offer policy recommendations based on these findings, as well as useful insights for researchers to better understand how the government is playing a role in linking materials research in academia and its eventual uptake in industry.

None and a Million – Challenges Identifying Just One Problem for a Platform Technology to Solve

Dr Daniel Mak[1,3,4], Dr Claude Meffan[1,2,3,4], Professor Renwick Dobson[1,3,4], Professor Volker Nock[1,3,4]
[1]University of Canterbury, Christchurch, New Zealand, [2]Victoria University of Wellington, Wellington, New Zealand, [3]Biomolecular Interaction Centre, Christchurch, New Zealand, [4]The MacDiarmid Institute for Advanced Materials and Nanotechnology, New Zealand

Session 7D: Science commercialisation, Dobson 3, February 12, 2025, 10:40 - 12:40

Platform technologies can transform multiple industries simultaneously by solving problems using the same underlying science and engineering. However, this is both a blessing and a curse as analysing multiple markets is arduous and time-consuming in the quest to find the ‘killer application’. Failure to focus on one application results in a lack of focus and ill-defined end-user requirements that affect the technological development.

Key challenges when assessing markets include access to experts, end-users, and customers, reliable metrics for comparison, varying technological requirements from each market, and ensuring the selected market has a genuine, valuable problem.

CapFlux uses capillary microfluidics to develop Lab-on-a-Chip diagnostic devices that can be faster, easier, and cheaper than alternative testing technologies while requiring zero electrical power and being hyper-portable. Initially branded as Winealyse, the initial application was the wine industry, but lack of demand has seen CapFlux faced with these challenges as it looks for future markets.

In this talk, Daniel will document his journey through these challenges and share the learnings from discussions with many experts. This will assist others going through the same process and motivate others to begin the process of engaging with end-users early.

Commercialisation of Carbon Free Alkalinity to Enhance the Removal of CO2

Dr Christopher Oze[1], Dr Megan Danczyk[1]
[1]Aspiring Materials, Christchurch, New Zealand

Session 7D: Science commercialisation, Dobson 3, February 12, 2025, 10:40 - 12:40

Climate remediation technologies commonly require a source of alkalinity. For example, utilizing rock alkalinity as an environmental addition has been proposed to remove atmospheric CO_2. Other technologies require alkalinity sources to neutralize acids. Silicate minerals/rocks are attractive sources of alkalinity due to containing no inherent carbon; however, rates of alkalinity enhancement from silicates are slow and limited. Additionally, challenges of adding silicates to the environment include high costs, exposure health risks, mining impacts, high water and energy consumption, and no accepted methodology to confirm that atmospheric CO_2 has been removed and stored. To address the alkalinity demand, a process developed by Aspiring Materials offers an engineered alkalinity source (i.e, Mg hydroxide) derived from silicate rocks. This approach provides several benefits: a direct and rapidly reactive alkalinity source, no contaminants (i.e., removed through processing), comparatively low water and energy consumption for CO_2 removal, and no CO_2 released from the source material or during processing. The benefits of Mg hydroxide as an alkalinity source and its ability to react with CO_2 are well established; however, a majority of Mg hydroxide is currently sourced from carbonates, contributing to CO_2 emissions. Aspiring Materials is scaling up to replace carbonate-derived alkalinity sources with those derived from silicates: supplying like for like products at a comparative cost and capable of offsetting megatonnes of CO_2.

Addressing the global plastics problem – value added adhesives derived from recycled plastics

Ibrar Hussain[1], Prof Matthew Watson[2]
[1]Nilo Ltd, Auckland, New Zealand, [2]University of Canterbury, Christchurch, New Zealand

Session 7D: Science commercialisation, Dobson 3, February 12, 2025, 10:40 - 12:40

Plastics are useful materials and will continue to be used for the foreseeable future. However, 400 million tonnes of waste plastics are generated every year. In addition, 15 million tonnes of urea formaldehyde, a recognised carcinogen, is used in the manufacture of wood fibreboard products every year.

NILO is well progressed in the development of an innovative process technology to address both these challenges by converting plastic waste into an adhesive to replace urea formaldehyde in the production of wood fibreboard. The patented Nilo technology can utilise all polyolefins (polyethylene and polypropylene) encompassing almost 60% of all plastic waste, including difficult to process soft plastic (film). The waste plastic derived adhesive produced via the NILO process has been tested at commercial scale and demonstrated to comply with the applicable engineering and quality standards.

In this presentation we will describe the journey of a small NZ-based start-up company, and the development of the plastics-to-adhesives process. Results of prototypical fibre-board properties be presented, alongside NILO’s future challenges.

Closing the loop: Circular Economy Strategies for Critical Materials in the Energy Transition

Dr Jim Goddin[1]
[1]Thinkstep-anz, Christchurch, New Zealand

Session 7D: Science commercialisation, Dobson 3, February 12, 2025, 10:40 - 12:40

The global transition to renewable energy is driving unprecedented demand for critical materials, such as lithium, cobalt, nickel, and rare earth elements, essential for technologies like batteries, wind turbines, and solar panels. However, reliance on these materials presents significant challenges, including supply chain risks, environmental degradation, and social implications. This paper explores the necessity of adopting "demand-led" circular economy principles to mitigate these issues. By focusing on sustainable mining, material efficiency, and recycling strategies, we can reduce our dependency on virgin materials, enhance economic resilience, and support a sustainable energy transition. This research outlines a pathway to achieving a circular model for critical materials in energy applications through a detailed analysis of current practices and future opportunities.

Dendritic Identifiers as Oracles in Agri-Food Supply Chains

Dr Michael Kozicki[1], Professor Mark Manfredo[1]
[1]Arizona State University, Tempe, United States

Session 7D: Science commercialisation, Dobson 3, February 12, 2025, 10:40 - 12:40

Contamination, waste, and food fraud cause significant product loss and economic damage in our global agri-food systems. Additionally, slow responses to outbreaks and economically motivated adulteration can impact public health. To combat these issues, Distributed Ledger Technologies (DLT), including permissioned blockchain with smart contracts, are increasingly being used to provide greater end-to-end visibility and information integrity. However, the chain of trust is only as strong as its weakest link, which, for the agri-food enterprise, is product labeling. Commonly used methods like printed alphanumeric strings, linear or two-dimensional barcodes, dot codes/QR codes, and graphics identify product type, origin, and quality but have two significant issues: (1) they are easy to forge or clone, leading to product misrepresentation, and (2) they are rarely individualized to specific items due to the costs associated with digital printing, resulting in a blanket approach to recalls and product loss due to poor supply chain intelligence. With the support of the USDA, we are developing an agri-food "oracle" – an element that securely connects trusted real-world data, in this case, item identity, with any DLT [1]. Our oracle is based on a novel secure and self-individualizing digital trigger called the Dendritic Identifier (DI), coupled with digital camera hardware and software [2]. The DI can be placed on labels, packaging, or directly on the item itself using a printing-like process and read using a cellphone, allowing trusted item-level information to be accessed through the supply chain, all the way to the consumer [3].

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Neuromorphic Computing – An Interdisciplinary Approach

Professor Rainer Waser[1]
[1]IWE2, RWTH Aachen University, Aachen, Germany

Session 7E: Neuromorphic unconventional and physical computing Symposium, Dobson 4, February 12, 2025, 10:40 - 12:40

In information technology, there is currently a transition from classical instruction-based computation, where algorithms are the recipes for data processing and lead to predictable results, to AI-based computation, which relies on machine learning and the automatic extraction of knowledge from data to produce results with a certain probability. The clear downside of this development is the enormous and increasing energy consumption of computing systems. For this reason, I will motivate my talk with the climate change.

In our projects, we are researching devices and systems for Neuromorphic Computing (NC) that are more energy-efficient than classical approaches. The focus of our research is on redox-based memristive elements. The word memristive reflects a combination of a memory and a resistor, so it is a resistor with (non-volatile) memory. It is generally believed that these elements represent a potential improvement beyond the limits of current memory technology in terms of write speed, write energy and scalability. In particular, they can provide an energy-efficient approach to NC concepts. However, it will be of big importance that energy saving is not counter-balanced by rebound effects.

In this talk, fundamental aspects of the physics of these elements will be briefly presented. Material physics will be linked to neighboring disciplines, neuroscience and computer science / artificial intelligence (AI). It will be shown that such an interdisciplinary approach brings the highest benefit in a future energy-efficient NC. In the outlook, we consider the implications of memristive-based NC and its potential impact on future AI. This will lead to aspects of advantages and threats by AI on a personal and societal level.

Brain-like data processing through multistable memristive circuits

Professor Ronald Tetzlaff[1], Dr. Ioannis Messaris[1], Dr. Ahmet Samil Demirkol[1], Professor Alon Ascoli[2], Professor Leon Chua[3]
[1]TUD Dresden University of Technology, Dresden, Germany, [2]Politecnico di Torino, Torino, Italy, [3]UC Berkeley, United States

Session 7E: Neuromorphic unconventional and physical computing Symposium, Dobson 4, February 12, 2025, 10:40 - 12:40

Upscaling from 2D chips to 3D structures for neuromorphic computing represent a challenge, especially when a level of complexity is reached that enables the processing of high-dimensional data in practice. In this context, memristive arrays for the implementation of analog computational methods or artificial intelligence structures have been investigated in a large number of publications. Particular attention has been paid to in-memory computing using crossbar arrays, neuromorphic networks and networks based on nonlinear dynamics. The latter have unprecedented computing power based on the dynamic behavior of interconnected, highly nonlinear memristive circuits and offer a new level of energy efficiency, i.e., they support the application of intelligent sensor-processor arrays of high complexity. Simulations and experiments have demonstrated that the memristors typically produced to date exhibit fading memory behavior, i.e., a single steady-state oscillatory solution that is independent of the initial state when excited by a periodic input.

In this paper, the development of multistable memristive structures is discussed in detail. Recent results show that multistability has been observed in both simulations and experiments for pulse-based and high-frequency sinusoidal inputs of different memristors.

Ferroelectric domain wall memory- From simple binary resistance switch to memristive properties.

Professor Nagarajan Valanoor[1], Dr Pankaj Sharma
[1]UNSW Sydney, UNSW Sydney, Australia, [2]Flinders University, Adelaide, Australia

Session 7E: Neuromorphic unconventional and physical computing Symposium, Dobson 4,
February 12, 2025, 10:40 - 12:40

Topological defects and structures that naturally form in crystalline solids with inherent or co-existing orders hold significant promise for advancing beyond von Neumann computing and data storage. Among these, ferroelectric domain walls—nanoscale interfaces that arise in materials with spontaneous polar order and can be controlled by electric fields—stand out as particularly promising for low-energy information storage and electronics.

This presentation will cover a series of milestones from our research program on non-volatile data storage using ferroelectric domain walls. These devices feature non-destructive reading at moderate voltages, high OFF-ON ratios, and excellent endurance and retention. Multi-state data storage is achieved by tuning wall length, selectively injecting or erasing domain walls with different charge states, and controlling the bending of isolated domain walls that opens avenues in “memristor” based information storage and processing.

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Understanding volatile threshold switching in metal-oxide-metal devices and its application as a solid-state neuron

Professor Robert Elliman[1]
[1]Australian National University, Canberra, Australia

Session 7E: Neuromorphic unconventional and physical computing Symposium, Dobson 4, February 12, 2025, 10:40 - 12:40

Two-terminal, metal-oxide-metal devices that exhibit volatile threshold switching, or current-controlled negative differential resistance, can be used to fabricate simple relaxation oscillators or leaky-integrate-and-fire neurons for use in neuromorphic computing. However, the specific response of devices depends on their size, structure and composition, as well as the conditions employed for their operation and measurement. Understanding such dependencies is critical for the effective application of threshold switching devices in neuromorphic computing.

This presentation draws on our recent studies of NbOx, VOx, VO2 and V3O5-based devices to elucidate some of these dependencies and demonstrate the utility threshold switching devices as oscillators and solid-state neurons [1-5]. Insight is provided by combining materials-characterisation, electrical characterisation and in-situ thermal imaging, with finite-element and lumped-element modelling of the devices. Specific examples will be presented to demonstrate the efficacy of this approach, including new insight into the electroforming process and the role of current localisation and insulator-metal transitions in threshold switching. Results from a recent study of V3O5-based devices [4,5] will also be presented to demonstrate the potential of photo-conductivity as the basis of a sensory neuron [5].

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(Cancer) Theranostics with (Intrinsically) Radiolabeled Nanomaterials

Professor Weibo Cai[1]
[1]University of Wisconsin - Madison, Madison, United States

Keynote Session 12, Auditorium, February 12, 2025, 13:40 - 14:15

Radiolabeled nanomaterials have gained tremendous interest over the last 2 decades, which can play diverse roles in imaging, image-guided drug delivery, as well as theranostics of a number of diseases such as cancer. Some recent examples of radiolabeled materials from our recent work will be briefly described in this talk.

Although chelator-based radiolabeling techniques (commonly used for labeling nanomaterials with radiometals such as 64Cu/89Zr) have been used for decades, concerns about the complexity of coordination chemistry, possible alteration of nanomaterial pharmacokinetics, and potential detachment of radioisotopes have driven the need for developing a simpler yet better technique for future radiolabeling, which may facilitate future clinical translation.

The emerging area of intrinsically radiolabeled nanomaterials can take advantage of the unique physical and chemical properties of well-selected inorganic or organic nanomaterials for radiolabeling, and more importantly, offer an easier, faster, and more specific radiolabeling possibility to facilitate future clinical translation. Generally speaking, the four major categories of intrinsically radiolabeled nanomaterials include: 1) hot-plus-cold precursors, 2) specific trapping, 3) cation exchange, and 4) proton beam activation.

Representative examples of these strategies will be briefly illustrated in this talk, with the main focus on our own work that involves the radiolabeling of a variety of nanomaterials via “specific trapping”. The nanomaterials investigated in our laboratory include silica/carbon-based nanomaterials, COVID-19 nano-vaccines, multifunctional/multimodal hybrid nanomaterials, iron oxide nanoparticles, micelles, DNA nanostructures, etc.

The physics and challenges of unconventional physical computing

Daniel Brunner[1]
[1]Cnrs / University Franche-Comte, Besancon, France

Keynote Session 14, Dobson 4, February 12, 2025, 13:40 - 14:15

Neural network (NN) concepts revolutionize computing by solving challenges previously thought to be reserved to the abstract intelligence of humans. However, the astonishing and substantial conceptual breakthroughs are so far not mirrored by advances in hardware specialized in physically implementing unconventional, non-Turing and non-symbolic computing. As always with computing, scalability is the key metric. Furthermore, for maximized efficiency, the largest fraction of a hardware should be dedicated to the core computational task, while auxiliary infrastructure should be pushed into the background. Finally, the programming or training step encompasses until now not fully understood consequences for such computing concepts. Neuromorphic and physical computing offers great opportunities in these aspects, and first breakthroughs are being made. I will provide an overview of the field and demonstrate our strategies to create the conditions of a new computing paradigm with real life applications.

Sonodynamic Therapy of Solid Tumors: From Small-Molecule to Targeted Nanomaterial Sonosensitizers

Professor Alejandro Sosnik[1]
[1]Technion-Israel Institute of Technology, Haifa, Israel

Session 8A: Medical nanotechnology and spectroscopy, Auditorium, February 12, 2025, 14:20 - 15:55

Cancer is among the leading causes of death worldwide and the most deadly disease in children above one year of age in Europe and North America. Most pediatric tumors do not hit adults as they originate from cells that have not undergone complete differentiation. Sarcomas represent 10% of the pediatric tumors.

Sonodynamic therapy (SDT) is a minimally invasive and localized anticancer therapy based on the in situ generation of reactive oxygen species (ROS) by combining low-intensity ultrasound (US), oxygen, and a sonosensitizer and it minimizes systemic toxicity. We designed and synthesized a novel type of hybrid amorphous TiO2/polymer nanomaterials that comprises the synthesis and aging of a Ti(IV)-acetone oxo-organo complex, its mixing with linear and branched amphiphilic poly(ethylene oxide)-poly(propylene oxide) block copolymers and their nanoprecipitation in water [1]. Nanoparticles can be produced with fine size control by changing the complex aging time and we demonstrated that they trigger cancer cell apoptosis in vitro [2]. Moreover, very recently, we demonstrated the ability of glucosylated hybrid nanoparticles to target tumors that overexpress glucose transporter-1 and improve their sono-dynamic anticancer activity in 2D and 3D tumor models in vitro and in vivo [3]. In this presentation, I will introduce the most recent advances in the field of SDT of cancer and the challenges standing ahead to translate this therapeutic strategy to the clinic.

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A New Class of Sulfoxide Polymer-Lipid Conjugates for stealth LNP

Miss On Ting Choy[1], Dr Nicholas Fletcher[1], Mr Mingdi Hu[2], Dr Changkui Fu[1], Prof Chunying Chen[2], Prof Andrew Whittaker[1]
[1]Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, Brisbane, Australia, [2]National Centre for Nanoscience and Technology, Beijing, China

Session 8A: Medical nanotechnology and spectroscopy, Auditorium, February 12, 2025, 14:20 - 15:55

Polyethylene glycol (PEG) functionalization is widely used in engineering nanocarriers to overcome physiochemical limitations and improve pharmacokinetic properties for enhanced delivery.[1] Despite the beneficial “stealth” properties of PEG, there are rising concerns around PEG immunogenicity, especially after broad exposure to mRNA COVID vaccines in general populations. A significant increase in anti-PEG antibodies following vaccination has been reported, and this is likely caused by accelerated system reactogenicity.[2] Anti-PEG antibodies have been broadly reported to affect the performance of PEGylated lipid-based delivery systems. Interestingly, research on developing alternative polymer-lipid conjugates to replace PEGylated lipids is rare, presenting an opportunity to introduce novel approaches to overcome this limitation.

Herein, we engineered new polymer-lipid conjugates, replacing PEG with a sulfoxide-containing polymer, a polymeric analogue of dimethyl sulfoxide (DMSO), with comparable physicochemical properties to serve as a “stealth” agent. In our approach, we first synthesized the polymer-lipid conjugates via reversible addition-fragmentation chain-transfer (RAFT) polymerization of 2-(methylsulfinyl)ethyl acrylate (MSEA) with a lipid chain transfer agent containing 1,2-distearoyl-sn-glycero-3-phosphorylethanolamine (DSPE). Polymer-lipid conjugate PMSEA-DSPE were incorporated into LNP formations and stability and shielding efficacy were screened. The utilized PMSEA mRNA-LNPs showed a higher transfection efficiency than the PEG counterpart, consistent with an enhanced endosomal escape profile. To provide further mechanistic understanding of engineered PMSEA materials, a second generation of PMSEA materials was produced. These were functionalized with carboxyl group for conjugation with biological targeting ligands to enhance specificity, as well as chelator ligands for quantitative PET preclinical imaging to observe pharmacokinetics and in vivo behaviours.

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Evaluation of Dynamic Light Scattering as a Potential Quality Control Method for Radiolabeled Antibody for Successful Tumor Detection

Huu Bao Nguyen[1], Hyun Park[2], Thuy Tien Nguyen[1], Kyeongwon Kim[1], Jeong Eun Lim[1], Jung Young Kim[2], Kyo Chul Lee[2], Dr Jeongsoo Yoo[1]
[1]Kyungpook National University School of Medicine, Daegu, South Korea, [2]Division of Applied RI, Korea Institute of Radiological and Medical Sciences, Seoul, South Korea

Session 8A: Medical nanotechnology and spectroscopy, Auditorium, February 12, 2025, 14:20 - 15:55

Background: Radiolabeled antibodies offer a powerful approach for cancer management, facilitating both nuclear imaging and radioimmunotherapy. However, the antibodies can be compromised during bioconjugation and radiolabeling, particularly due to radiolysis. The current standard quality control, size-exclusion high-performance liquid chromatography (SEC-HPLC), may not detect all components, particularly aggregates. This study explores the use of dynamic light scattering (DLS) as a novel quality control method to detect aggregation that is undetectable by conventional SEC-HPLC.

Methods: Trastuzumab was subjected to bioconjugation with p-NCS-Bn-NOTA chelator and radiolabeling with [64Cu]CuCl2 . DLS analysis was performed at each step, both before and after purification, and the results were compared with SEC-HPLC data. Based on DLS data, purification methods were optimized. The impact of aggregation on in vivo tumor uptake was evaluated through biodistribution studies and positron emission tomography (PET) imaging, assessing the correlation between aggregation levels and tumor-targeting efficacy of the radiolabeled antibodies.

Results: DLS analysis revealed ~25% aggregation peak during bioconjugation of trastuzumab, which increased to nearly 50% following radiolabeling. This aggregate was almost removed after three rounds of centrifugal filtration. In vivo tumor targeting demonstrated a strong correlation between reduced aggregation and increased intact antibody, with a Pearson’s correlation coefficient exceeding 0.7.

Conclusion: The study highlights the significance of monitoring aggregation during antibody bioconjugation and radiolabeling processes, which is often undetected by SEC-HPLC. The findings suggest that DLS, as a rapid and convenient method, holds promise as a quality control tool for radiolabeled antibodies in both preclinical and clinical settings.

Enhanced UV-B Emission in BaB8O13: Optimizing Gd3+ Doping with Pb2+, Ce3+, and Pr3+ for Phototherapy Applications

Professor Leelakrishna Reddy[1]
[1]University of Johannesburg, Dooornfontein, South Africa

Session 8A: Medical nanotechnology and spectroscopy, Auditorium, February 12, 2025, 14:20 - 15:55

We present an intriguing scenario involving a wide band gap (4.3 to 4.5 eV) semiconducting material, BaB8O13, which serves as an ideal host for embedding rare-earth ions such as gadolinium (Gd3+). Gd3+ ions typically require high excitation energy, generally above 250 nm, to transition from their ground state to a higher excited state. BaB8O13 is particularly well-suited for this purpose as it can effectively absorb energy and transfer it to the embedded Gd3+ ions, resulting in emissions in the UV-B range around 311 nm. To further enhance emissions at approximately 311 nm, the host material can be co-doped with sensitizers such as Pb2+, Ce3+, and Pr3+. These sensitizer ions absorb the excitation energy and transfer them non-radiatively to the Gd3+ ions, thereby amplifying the emissions in the UV-B range. This process controls the efficient energy transfer mechanisms between the host lattice and the embedded ions, which is crucial for maximizing the emission intensity. These UV-B emissions are particularly significant for phototherapy, as they fall within the action spectrum for the treatment of various skin conditions such as psoriasis and vitiligo and many more. Additionally, the ability to fine-tune the emission properties through co-doping strategies with Gd3+ as a UV-B emitting source opens possibilities for optimizing the material for specific therapeutic applications. The development of such materials could lead to more efficient and targeted phototherapeutic treatments, reducing exposure times and improving patient outcomes.

Synchrotron-Based Characterization of Advanced Materials: From Structure to Function

Dr Qinfen Gu[1]
[1]Australian Synchrotron, ANSTO, Clayton, Australia

Session 8B: Synchrotron-based methods for materials science and engineering, Dobson 1, February 12, 2025, 14:20 - 15:55

The energy crisis and environmental degradation, including pollution, climate change, and resource depletion, represent major challenges of the 21st century. As demand for finite resources grows, finding sustainable solutions is more urgent than ever. One promising solution is the development of new batteries that can meet energy needs while also benefiting the environment. Synchrotron radiation provides powerful beams for in-situ analysis of advanced materials. Techniques such as in-situ X-ray diffraction (PXRD), small-angle X-ray scattering (SAXS), and X-ray absorption spectroscopy (XAS) offer critical insights into material behavior, driving progress toward clean, renewable energy solutions. This presentation will delve into these developments.

the XAS Beamline in Melbourne: 100% Efficient and Awesomely Fast

Dr Bernt Johannessen[1]
[1]Australian Synchrotron, ANSTO, Clayton, Australia

Session 8B: Synchrotron-based methods for materials science and engineering, Dobson 1, February 12, 2025, 14:20 - 15:55

Synchrotron techniques can broadly be categorised into two types. One is used to collect “an image” at a fixed energy, such as X-ray powder diffraction (PD), and another to collect “an image” across multiple energies to build up a complete spectrum, such as X-ray absorption spectroscopy (XAS). XAS is a versatile technique for probing oxidation states and local atomic structures in a wide range of samples, including solids, liquids, nanoscale, and single-atom materials. The XAS Beamline at the Australian Synchrotron in Melbourne has seen increasing demand, particularly from the catalysis and energy storage research communities [1, 2], creating pressure on accessibility.

This presentation will first provide an update on the Australian Synchrotron’s facility status and the techniques available. It will then explore recent developments at the XAS Beamline, particularly the implementation of slew scanning techniques, which enable entire XAS spectra to be collected in approximately 10 seconds – comparable to the scan rate at fixed energy "imaging" beamlines. These advancements are expected to alleviate some of the demand pressures, enhancing our ability to contribute to cutting-edge scientific investigations.

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Refining structures of electrochemical catalysts for energy storage and conversion

Dr Jinqiang Zhang[1]
[1]University of Technology Sydney, Sydney, Australia

Session 8B: Synchrotron-based methods for materials science and engineering, Dobson 1, February 12, 2025, 14:20 - 15:55

The development of highly efficient catalysts to improve the electrochemical performances is urgently needed due to the ever-increasing demand for energy storage and conversion devices in the last few decades. However, the electrochemical performances are still not satisfying to be potentially used in industrial applications. Here, we present our recent research on the structure tuning for electrocatalysts designed for energy storage and conversion devices such as Li-O2 batteries and electrochemical water splitting.1-5 We show that by carefully designing and tailoring the molecular and electronic structures, the efficiency of the applied catalysts could be maximized which would be highly beneficial for the electrochemical performances in their individual applications. For instance, TEMPO-modified ionic liquid could stabilize the lithium anode and prolong the cycle life of Li-O2 battery,2 while in-situ exfoliated MXene coupled with single Pt atoms show a mass activity more than 40 times higher than the commercial Pt/C.4 All these provide theoretical and experimental guidance to develop highly efficient catalysts for energy storage and conversion devices in the future.

Facile dissociation of molecular nitrogen on crystalline lanthanide surfaces

Dr Kiersten Kneisel[1], Dr. Jay Chan, Dr. Caitlin Casey-Stevens, Associate Professor Anna Garden, Dr. William Holmes-Hewett, Associate Professor Ben Ruck, Associate Professor Franck Natali, Emeritus Professor Joe Trodahl
[1]Victoria University of Wellington, Wellington, New Zealand

Session 8B: Synchrotron-based methods for materials science and engineering, Dobson 1, February 12, 2025, 14:20 - 15:55

Keywords: lanthanide, lanthanide nitride, synchrotron spectroscopy, density functional theory, molecular dynamics, Anderson impurity model

The dissociation of the strong triple molecular nitrogen (N2) bond is one of the rate-limiting steps in the Haber-Bosch process for ammonia production. This process requires high temperatures and pressures and accounts for ~2% global energy consumption and ~1.3% of CO2 emissions [1]. The N2 bond is broken with surprising ease by lanthanides which spontaneously form lanthanide nitrides under ambient conditions [2, 3].

We explore this reaction by combining experimental data with various computational techniques to develop a multi-faceted model. Experimental results from an in-situ study conducted at the Australian synchrotron on incrementally nitrided gadolinium and samarium thin films using x-ray photoelectron spectroscopy (surface sensitive) and x-ray absorption spectroscopy (bulk sensitive) will be discussed. These results are compared with density functional theory density of states calculations, ab initio molecular dynamics simulations, and Anderson impurity model calculations. The resulting model of lanthanide nitride formation is an important step towards developing a microscopic understanding of the catalysis, vital in developing a low energy ammonia production process.

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Understanding mechanically-activated changes during additive manufacturing

Professor Ronan Daly[1], Erica Watchorn-Rokutan[1], Dr Susannah Evans[1], Dr Niamh Willis-Fox[1,2], Dr Etienne Rognin[1]
[1]Department of Engineering, University of Cambridge, Cambridge, United Kingdom, [2]University of Manchester, Manchester, United Kingdom

Session 8C: Additive manufacturing and printing, Dobson 2, February 12, 2025, 14:20 - 15:55

This presentation explores the highly controllable and repeatable velocity gradients and forces experienced in additive manufacturing processes such as inkjet printing and extrusion-based additive manufacturing and how this can influence functional and biological materials being printed. Printing is a key tool when developing flexible process technologies. It is anticipated to be an important enabler for more personalised tissue engineered products and also drug delivery systems, where manufacturers can target tailor-made doses, drug release characteristics and combinations of drug compounds focused on individual needs [1]. With a steady growth of more targeted biopharmaceuticals, printing is also seen as an important technology to help address the inherently more costly development and manufacturing [2].

Here, we firstly present a study to better understand the overall printing process and the range of negative influences that can occur during bioprinting. We then examine the nozzle flow in particular and present custom-made experimental techniques to precisely control the forces experienced by solutions and hydrogels within nozzles and study how this can allow us to deliberately protect materials or drive chemical changes. Finally, we present how targeted chemical reactions can be achieved in additive manufacturing nozzle flows using mechanical forces alone to activate stress-sensitive functional molecules embedded within a polymer chain, in a field known as polymer mechanochemistry [4]. These stress-sensitive 'mechanophores' have been extensively studied at the molecular level but there have only recently been steps to understand how they react when included in additive manufacturing techniques or translated into real applications [5,6].

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3D printed plug flow reactor in space? Catalytic decomposition of a green propellants.

Dr Simon Reid[1], Dr Frédéric Lecarpentier[2], Associate Professor Digby Symons[3], Professor Matthew Watson[4]
[1]Aspiring Materials, Christchurch, New Zealand, [2]Advanced Engineering and Materials Team, Callaghan Innovation, Wellington, New Zealand, [3]Department of Mechanical Engineering, University of Canterbury, Christchurch, New Zealand, [4]Biomolecular Interaction Centre and Department of Chemical and Process Engineering, University of Canterbury, Christchurch, New Zealand

Session 8C: Additive manufacturing and printing, Dobson 2, February 12, 2025, 14:20 - 15:55

Concentrated hydrogen peroxide (high-test peroxide, HTP) belongs to a class of liquid rocket propellants used for low-to-medium thrust applications. HTP has similar performance yet significantly reduced toxicity when compared to hydrazine, and demand is increasing for HTP as a green alternative.

Central to HTPs use is the catalyst bed, housed in a plug flow reactor, and used to decompose hydrogen peroxide into steam and oxygen gas. An idealised catalyst will have a low pressure drop, high capacity, fast thermal response, and survive many thermal cycles over its lifetime. The incumbent catalyst and its architecture (silver supported on wire mesh) falls short of the ideal, and to date no other catalyst has been widely adopted for HTP decomposition.

Issues of high pressure drop and low decomposition efficiency might be solved through the adoption of novel catalyst supports (manufactured via 3D-printing). However, the advantages of such catalysts over traditional supports have yet to be validated experimentally. In this presentation, catalysts based on the Schoen Gyroid triply periodic minimal surface (TPMS) were printed and tested alongside their traditional counterparts in a thruster-type setup. Our results indicate that at equal surface area, Schoen Gyroid catalysts have a higher decomposition capacity than extruded honeycombs and a lower pressure drop than randomly packed spheres. Partial validation of an existing reactor model also highlighted the strong influence of the geometry on the catalyst performance. Therefore, HTP thrusters may benefit from the gyroid and other such novel catalyst supports, that, before 3D-printing, were impossible to manufacture.

Development of Advanced Biobased Materials: PHA-Plant Biomass Composites for 3D Printing Applications

Dr Yi Chen, Dr Claire Mayer-laigle[1], Nathan Hindenoch[2], Edwidge Audibert[3,5], Rob Whitton[2], Frederic Martel[3], Johnny Beaugrand[4], Christophe Collet[2], Caroline Rémond[5], Gabriel Paes[5], Maxime Barbier[2], Marie Le Guen[2]
[1]IATE- INRAE, Université de Montpellier, Institut Agro, Montpellier, France, [2]SCION, Rotorua, New Zealand, [3]Européenne de Biomasse, Pomacle, France, [4]BIA - INRAE, Nantes, France, [5]FARE - INRAE, Université de Reims Champagne Ardenne, Reims, France

Session 8C: Additive manufacturing and printing, Dobson 2, February 12, 2025, 14:20 - 15:55

Our current lifestyle and technological advancements drive societal expectations for the design of new high-tech products. However, the urgency of the climate crisis and the depletion of fossil fuel resources necessitate developing these products within a bioeconomy framework. Biobased materials offer one of our best alternatives. Yet, the properties of these materials often differ significantly from those of traditional materials, making them challenging to process using advanced technologies like additive manufacturing. This is particularly true for polyhydroxyalkanoates (PHAs), microbial biopolymers that are promising due to their excellent biocompatibility, biodegradability, and low environmental impact. However, their crystallization behavior, which depends on temperature and processing conditions, complicates their use in traditional 3D printing processes[1].

The work presented here focused on developing formulations and preparation processes for PHA composites—reinforced with biomass fillers in the form of powders and filaments—intended for printing using selective laser sintering (SLS) [2, 3] and fused deposition modeling (FDM)[4], respectively. The addition of biomass powders with specific physical properties (size, shape) and biochemical compositions influences the rates of hot and cold crystallization, enabling, on the one hand, the development of composite particles for SLS printing and, on the other hand, reducing warping phenomena, thereby facilitating the printing of complex objects by FDM. This work, which is the subject of two patents, opens up exciting prospects for the development of bio-based technical materials compatible with the applications of tomorrow.

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Optimizing material use with high-precision capillary printing for electronic device fabrication

Ms Jessica Tournaud[1], Ms Tanisha Badhauria[1,2], Ms Jamie Silk[1], Dr Gustavo Ardila[2], Dr David Riassetto[1], Dr Céline Ternon[1]
[1]Univ. Grenoble Alpes, CNRS, Grenoble INP, LMGP, Grenoble, France, [2]Univ. Grenoble Alpes, CNRS, Grenoble INP, Croma, Grenoble, France

Session 8C: Additive manufacturing and printing, Dobson 2, February 12, 2025, 14:20 - 15:55

Nowadays, an increasingly connected lifestyle is encouraged by a competitive global electronics industry that disregards its environmental impact. In fact, little attention is currently paid to raw material resources or end-of-life recycling and reuse opportunities, whether at the beginning or end of the electronic device life cycle. It is increasingly recognized that the dominant linear model of "take, make, use, and dispose" generates unsustainable waste that could and should be controlled throughout the life cycle of electronic and electrical products. Products designed to last longer, as well as greater recovery, reuse, and recycling of electronic waste, will reduce demand for source materials, packaging, and transportation. However, some sectors require single-use electronic products for critical safety criteria to avoid cross-contamination of medical products or in the case of smart packaging. For these applications, a mindset shift in design is necessary. The environmental impact of chosen materials and processes, including end-of-life, must be considered from the design phase.

In the present work, we develop a process flow based on high precision capillary printing [1] to build devices based on ZnO nanonets which are two-dimensional networks of randomly oriented ZnO nanowires. The printing step is not only used for the silver electrode design but also for patterning the device through etching. Comparison with results from devices fabricated with standard microelectronic processes are given.

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The use of cellulose in additive manufacturing (3D printing) and thermoforming.

Mrs Erica Sue-Tang[1]
[1]Lincoln Agritech Limited, Christchurch, New Zealand

Session 8C: Additive manufacturing and printing, Dobson 2, February 12, 2025, 14:20 - 15:55

Microplastics have become a worldwide problem found in food, water 1, and throughout the organs of the human body 2. Perhaps most terrifyingly, this includes breast milk 3. Some studies suggest the association of cardiovascular disease and low male fertility with microplastics but overall, the effect of microplastics is only recently being investigated. Microplastics are caused by the breakdown of non-biodegradable plastics. Single-use plastics are a big contributor to this. New Zealand legislation has introduced a phased ban on single-use plastics 4 from 2019-2025. This includes bio-based plastics such as PLA which does not degrade in the environment and causes similar harm to conventional plastics.

At Lincoln Agritech, we have developed a process that creates a plastic-like material from cellulose, using plant sources such as wood pulp and hemp. Use of Native New Zealand sources of cellulose such as Tawa, Harakeke, and Cabbage Tree inspired by Mātauranga Māori are among the long-term goals of this project. All chemicals used to make this plastic can be recovered and reused, creating a closed-loop process. The plastic-like properties indicate that this product can be used in conventional manufacturing methods such as 3D printing and thermoforming. It has the potential to replace single-use plastics currently on the market today.

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Mechanical testing of human endometrial tissue towards modelling the invasive behaviour of endometriosis.

Katherine Ellis[1,2], Dr Jacqueline Donoghue[3], Dr Rachael Wood[1]
[1]University of Canterbury, Christchurch, New Zealand, [2]Endometriosis New Zealand, Christchurch, New Zealand, [3]University of Melbourne, Melbourne, Australia

Session 8D: Tissue engineering and analysis, Dobson 3, February 12, 2025, 14:20 - 15:55

It is well established that the stiffness of the mechanical microenvironment of the cell has an influence on a range of cellular behaviours including morphology, gene expression, rate of proliferation, and invasiveness (1-3). Disruptions in the mechanical contractility of the uterus have been proposed as a potential factor in the development of endometriosis, as patients with this condition display abnormal, more intense uterine contractions compared to healthy individuals (4,5). Endometriosis involves the presence of endometrial-like cells outside the uterus and endometrial cells are known to alter their mechanical properties during the invasive process of trophoblast implantation (6). Therefore, we hypothesized that differences in uterine stiffness between individuals with and without endometriosis might explain the mechanisms that allow invasion to occur. There are several examples in cancer research where the mechanical environment has been targeted for successful treatment (7), paving the way for a similar potential therapy for endometriosis.

In collaboration with the Royal Women's Hospital in Melbourne, we took tissue from endometriosis patients and took measurements for Youngs modulus (AFM) and the Storage modulus (rheology). These values were compared against endometrial tissue from patients without endometriosis. By directly comparing the stiffness of the tissue between patients with and without endometriosis, we can begin to understand how the disease is able to invade and progress, and therefore explore targets for treatment.

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Designing Light-activated Hydrogels for Biofabrication of Complex Tissues and Biointerfaces

Professor Tim Woodfield[1], Dr Max Yavitt[1], Dr Axel Norberg[1], Dr Gretel Major[1], Dr Bram Soliman[2], Ms Laura Veenendaal[1], Ms Melissa Ishii[1], Dr Gabriella Lindberg[3], Dr Xiaolin Cui[4], Associate Professor Khoon Lim[5]
[1]University of Otago Christchurch, Christchurch, New Zealand, [2]University of New South Wales, Sydney, Australia, [3]University of Oregon, Eugene, USA, [4]Chinese University of Hong Kong (Shenzen Campus), Shenzen, China, [5]University of Sydney, Sydney, Australia

Session 8D: Tissue engineering and analysis, Dobson 3, February 12, 2025, 14:20 - 15:55

Biofabrication technologies, including extrusion bioprinting, bioassembly, digital light processing (DLP) and volumetric bioprinting (VBP), offer the potential to engineer constructs consisting of cell-laden bioinks, tissue modules, and/or bioactive factors that replicate the complex 3D organization of native tissues. Despite rapid advances however, development of individual bioinks for each biofabrication technique and specific tissue niche is required, limiting rapid innovation and scalability for advanced biological applications. Our overall goals are to address major bottlenecks that remain in designing materials that are both cell-instructive and compatible with high resolution 3D biofabrication techniques.

This talk discusses alternative strategies to engineer highly tuneable hydrogel platforms that: 1) promote a specific cell-instructive niche using visible-light photocrosslinking in gelatin-based hydrogels, bioresins and high-throughput microgels, and 2) are printable across multiple different biofabrication technologies.
We describe design of a versatile photoinitiator system (Ru/SPS) and photo-clickable gelatin-based bioinks for biofabrication of 3D in vitro models. Tailoring macromolecular chemistry (eg allylated-gelatin hydrogels; GelAGE), we engineer the cell-instructive tissue niche for multiple cell types via: covalent incorporation of thiolated bioactives (eg heparinSH); delayed dissolution sacrificial bioinks; tailored stiffness gradients in cell-laden microgel filaments fabricated using a microfluidics approach, as well as di-tyrosine cross-linking of native decellularized extracellular matrix (dECM) based bioinks for volumetric tissue analogues in centimetre scale. Examples discussed include engineering human stem-cell microenvironments for cartilage/bone regeneration, disease modelling, vascular network formation, and human lipoaspirate grafts.

This work demonstrates advances in engineering of cell instructive universal bioink platforms for 3D bioprinting and high-throughput screening, and advances scalable biofabrication of 3D biological models and functional tissues.

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Stiffness Patterning hydrogels to engineer stem cell-derived cardiac scar tissue for disease modelling

Mr Harrison Porritt[1,3], Dr Annika Winbo[4], Prof. Andrew Taberner[2], Dr Amatul Mateen-ahmad[4], Dr Alex Dixon[2], Assoc. Prof. Jenny Malmström[1,3]
[1]Department of Chemical and Materials Engineering, University of Auckland, Auckland, New Zealand, [2]Auckland Bioengineering Institute, Auckland, New Zealand, [3]The MacDiarmid Institute for Advanced Materials and Nanotechnology, Auckland, New Zealand, [4]Faculty of Medical and Health Sciences, Physiology, Auckland, New Zealand

Session 8D: Tissue engineering and analysis, Dobson 3, February 12, 2025, 14:20 - 15:55

The extracellular matrix (ECM) impacts cell and tissue physiology. Significant changes in ECM composition occur post-heart attack during scar formation. Dying tissue is stabilised by the overproduction of ECM proteins from activated fibroblasts (myofibroblasts), stiffening the tissue and preventing tissue rupture. Complications can occur when the stiffer less compliant scar tissue puts excessive strain on healthier regions, resulting in heart failure [1].

This project uses a tissue engineering approach to create a 3D physical system that mimics the boundary between healthy cardiac and cardiac scar tissue. Induced pluripotent stem cells (IPSC) derived cardiomyocytes (CM) and fibroblasts are encapsulated within stiffness-patterned Gelatin methacryloyl (GelMA) hydrogels. Modulation of the stiffness spatially creates regions of healthy and fibrotic tissue by controlling fibroblast differentiation into myofibroblasts, activated through mechanotransduction pathways [2].

This presentation will show the capabilities of our current system to control fibroblast activation in stiffness-patterned hydrogels. Highlighting the ability to spatially control the stiffness over a single gel, from >10 kPa (healthy) to ~45 kPa (fibrotic stiffness) over the range of 10 µm using a custom-built light projector setup [3]. It will also show the ability of this system to encapsulate co-cultures of CMs and cardiac fibroblasts, with adequate cell viability, creating 3D cell-laden structures. Highlighting the ability to spatially control fibroblast differentiation into myofibroblasts within the stiffness-patterned gels through increased fibroblast size and the presence of smooth muscle actin. This research will further the knowledge of scar formation and contribute to discovering possible treatments for scar regression.

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Harnessing oxygen availability to fabricate advanced biological materials for tissue engineering applications

Dr. Axel Norberg[1], Melissa Ishii[1], Dr Axel Norberg[1], A/Prof. Khoon Lim[2], A/Prof. Gabriela Lindberg[3], Prof. Tim Woodfield[1]
[1]University Of Otago, Christchurch, New Zealand, [2]University of Sydney, Sydney, Australia, [3]University of Oregon, United States

Session 8D: Tissue engineering and analysis, Dobson 3, February 12, 2025, 14:20 - 15:55

Spatiotemporal control over oxygen availability is crucial for the generation of advanced biological materials used in tissue engineering (TE) applications. Sufficient oxygen concentrations are required for cell survival, yet effective oxygen diffusion is limited within tissue constructs larger than a few millimeters [1]. Conversely, the presence of oxygen inhibits radical polymerization, which is an effective method to prepare polymer-based biological materials, such as hydrogels [2]. Thus, the tradeoff between promoting cell survival or achieving predictable material properties presents challenges to fabricating complex and physiologically relevant biological materials for TE applications. In this work, we present two unique technologies enabling spatiotemporal control over oxygen availability to promote enhanced cell survival and improve material properties in large TE constructs. In one strategy, we harness the decomposition of calcium peroxide (CaO2) to generate molecular oxygen inside gelatin-based microparticles. Assays for cell viability and functional biological outputs show that controlled spatial assembly of CaO2 microparticles increases local oxygen concentrations and mitigates the cytotoxic effects of CaO2 decomposition to promote cell survival. In the second strategy, we utilize the decomposition reaction of sodium sulfite (Na2SO3) to deplete molecular oxygen in hydrogel scaffolds. Rheology experiments show that the removal of oxygen prevents oxygen inhibition of radical polymerization to improve hydrogel mechanical properties. We then exploit this phenomenon to fabricate more mechanically robust and cytocompatible tissue constructs using 3D bioprinting of light-activated polymers. These results highlight novel approaches to harness spatiotemporal oxygen availability for the generation of advanced biological materials.

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A multiscale approach for plasmo-electronic effects in self-assembled gold nanoparticle networks

Dr Louis Merle[1], Dr Adnen Mlayah[2], Dr Jeremie Grisolia[1]
[1]LPCNO CNRS/INSA TOULOUSE, Toulouse, France, [2]LAAS/CNRS, Toulouse, France

Session 8E: Neuromorphic unconventional and physical computing Symposium, Dobson 4, February 12, 2025, 14:20 - 15:55

Self-assembled metallic nanoparticles surrounded by organic ligands display plasmoelectronic effects, which can manifest as either positive or negative photoconductance. Such complex phenomena comes from the linkage between charge transport and surface plasmons in metal nanostructures that might thus serve as a synaptor depending on their stimulation, which is particularly interesting for neuromorphic circuits. Here, we present a multi-scale modeling of the plasmo-electronic properties of self-assembled monolayers of colloidal gold nanoparticles (NPs). We particularly address the dynamical conduction characteristics of the electrical paths in response to optical excitation. Impedance spectroscopy measurements performed under optical stimulation are utilized to evaluate the plasmo-electronic characteristics of the NP assembly in relation to laser irradiation intensity and wavelength. The role of the surface plasmon resonance is especially highlighted. The impedance spectroscopy data are analyzed using a multi-scale approach in which a local nano-junction model, composed of parallel inter-particle resistance Rij, capacitor Cij and photo-resistance gij-1, serves as a building block of the electrical network. The interparticle photo-conductance gij is calculated using electro-dynamic simulations based on the discrete dipole approximation (DDA) and accounts for the local plasmonic properties. The electric characteristics of the macroscopic circuit formed by the nano-junctions network are calculated using a numerical resolution of current-voltage system based on Kirchhoff's laws. The results of DDA-Kirchhoff numerical simulations are compared quantitatively to the experimental data. The findings shed light on the plasmo-electronic properties of self-assembled nanoparticle networks at multi-scale (macro to nano), as well as the evolution of electrical paths in response to laser excitation.

Energy efficient, scalable, self-formed Ag nanostructure based neuromorphic devices exhibiting high degree of linearity for In-memory computing

Professor Giridhar Kulkarni[1]
[1]Jawaharlal Nehru Centre for Advanced Scientific Research (jncasr), Bengaluru, India

Session 8E: Neuromorphic unconventional and physical computing Symposium, Dobson 4, February 12, 2025, 14:20 - 15:55

The human brain, comprising nearly a hundred billion neurons with several orders higher numbers of synapses, accomplishes massive parallel processing and unmatched cognitive actions. Inspired by this, global efforts are ongoing to develop artificial neural networks to emulate human intelligence, leveraging complex algorithms on current high-speed computational platforms. However, when tackling complex real-world problems, which the biological brain handles effortlessly in real-time, even the most advanced computers face challenges due to high energy consumption and limitations in data processing speed. In contrast, biological synapses manage both processing and memory parallelly, linked to their adaptability, known as neuroplasticity. Although the complexities involved are still being explored, research is progressively focusing on replicating various levels of neuroplasticity using artificial synaptic devices with emphasis on low-energy devices [1].

This presentation covers the literature on this topic, with emphasis on self-forming device recipes. A self-formed labyrinth structure of Ag, scalable over cm2 areas [2], mimicking neuronal bodies and axonal network connectivity, has been explored in the laboratory and the outcome of the study will be described. This interesting device architecture enabled us to emulate using voltage spike signals, basic to complex synaptic activities, importantly, without the aid of external circuitry [3,4]. Another important feature is the linear updating of the synaptic weight (both conductance and its retention), which facilitated in-memory computation. Specifically, arithmatic operations with random pulsing sequences, effective pulse pairing to achieve complicated math operations such as progression, have been achieved with minimal energy consumption (1fJ/synapse).

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Critical oscillator networks for reservoir computing applications

Dr Petro Feketa[1], Bakr Al Beattie[2], Karlheinz Ochs[2], Thomas Meurer[3], Hermann Kohlstedt[4]
[1]Victoria University of Wellington, Wellington, New Zealand, [2]Ruhr-University Bochum, Bochum, Germany, [3]Karlsruhe Institute of Technology, Karlsruhe, Germany, [4]Kiel University, Kiel, Germany

Session 8E: Neuromorphic unconventional and physical computing Symposium, Dobson 4, February 12, 2025, 14:20 - 15:55

In this talk, we will explore two case studies of oscillator networks within the framework of reservoir computing: spin-torque nano oscillators and ensembles of FitzHugh-Nagumo oscillators. By analysing these networks, we will investigate the relationships between their criticality properties and performance in classification tasks. Specifically, we will demonstrate how operating at or near criticality can significantly enhance the robustness and accuracy of classification, particularly in scenarios where the readout layer is subject to dimensional reduction [1]. The criticality property, characterised by the system's balanced state between order and disorder, is shown to be an important factor in maintaining high levels of computational performance despite constraints on the readout layer. Furthermore, we will discuss the macroscopic properties of the interconnection topology of these networks. By examining the structural configurations of the oscillator networks, we aim to highlight their essential role in system's criticality and, consequently, its effectiveness within a reservoir computing framework [2]. Our discussion will provide insights into the design principles for oscillator networks for reservoir computing applications, underscoring the importance of criticality and network topology. This analysis is not only relevant for understanding fundamental aspects of complex systems but also for advancing practical implementations in computational paradigms that leverage the inherent dynamics of physical systems for information processing tasks.

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Cost-effective fabrication of advanced thermal management materials for high-power electronic devices

A/Prof Fei Yang[1]
[1]University of Waikato, Hamilton, New Zealand

Session 9A: Thermal management and materials, Auditorium, February 12, 2025, 16:25 - 17:50

The technical capabilities of modern electronic devices increasingly demand higher frequencies, more power, and greater miniaturization. Rapid heat dissipation is critical to ensuring these high-power devices maintain function and avoid overheating. Developing advanced thermal management materials with high thermal conductivity and cost-effective manufacturing technology is of significant global interest. In this presentation, I will present a cost-effective route to produce advanced copper-matrix composite heat-sink materials, which have potential to be used in high-power electronic components; and discuss the key affecting factors that influence the composite's heat transfer behaviors.

Optimizing Thermal Conductivity and Mechanical Properties of Hot-pressed Copper-Titanium/Diamond Composites

Miss Jingnan Ma[1], Dr. Rob Torrens[1], A/Prof Leandro Bolzoni[1], A/Prof Fei Yang[1]
[1]University of Waikato, Hamilton, New Zealand

Session 9A: Thermal management and materials, Auditorium, February 12, 2025, 16:25 - 17:50

The development of heat sink materials is essential for efficiently dissipating the heat generated by increasingly integrated and miniaturized electronic devices. Copper/diamond composites are promising candidates due to the excellent thermal conductivity (TC) of both copper matrix and diamond. To address the poor chemical affinity between copper and diamond, this study added titanium powder in amount of 0.3 wt.%, 0.5 wt.%, and 0.7 wt.% to the copper matrix. The copper matrix composites reinforced with 50 vol% diamond particles were prepared by hot pressing at 1050 °C. The Cu-0.5 wt.%Ti/diamond composites achieved the highest TC of 546 W/mK and tensile strength of 97 MPa. This is attributed to the formation of a uniform and thin TiC interface with the addition of 0.5 wt% titanium, thereby modifying the large gap in acoustic impedance between copper and diamond and improving the interfacial bond strength. However, with the increase in titanium content to 0.7 wt%, the thickness of TiC interface significantly increases, leading to a substantial reduction in the TC of the composites attributed to the intrinsic low TC of TiC and the interface de-bonding with a thicker TiC interface. This study provides a cost-effective method for fabricating copper/diamond composites and offers insights into designing copper-titanium/diamond composites with high TC for heat sink materials.

Thermal characterisation of cFET Stability

Mr Rhys Marchant-ludlow[1], Zhuoyue Wang[1], Dr Daniel Mak[1], Professor Renwick Dobson[1], Dr Volker Nock[1]
[1]University Of Canterbury, Christchurch, New Zealand

Session 9A: Thermal management and materials, Auditorium, February 12, 2025, 16:25 - 17:50

The capillary field effect transistor (cFET), developed at the University of Canterbury1-3, has been instrumental in furthering flow control in capillary microfluidic devices4-7. In its basic form, the cFET works by expanding a volume of air into a channel, cutting off liquid flow in the process. This is useful for automation within microfluidic chips and for precise control of liquid volumes. However, the thermal stability of the cFET has yet to be characterised, leaving its performance under varying environmental temperatures uncertain. This study addresses that gap by integrating thermal probes into a custom-designed chip to monitor air- and liquid-temperature within the cFET structure, and the material temperature of the overall chip. Rhodamine B, a temperature-sensitive fluorescent dye8, is used as the sensor fluid within the chip. Using the thermal probes, the fluorescence of the Rhodamine B can be characterised, allowing further thermal experimentation of cFETs to be performed without the need for intrusive macro-scale probes. Based on preliminary findings, we hypothesise that increasing temperature will improve cFET closing through thermal expansion of the air volume, whereas decreasing temperature will lead to the opposite. The extent of these temperature-induced effects still needs to be characterised. This research is significant as it will determine whether the cFET can be used for thermally actuated assays, such as DNA sequencing on a chip, potentially vastly increasing the number of applications it can be used in.

Development and characterization of novel and stable nanoparticles embedded PCM-in-water emulsions for thermal energy storage

Dr Sunil Lonkar[1]
[1]Technology Innovation Institute, Abu Dhabi, United Arab Emirates

Session 9A: Thermal management and materials, Auditorium, February 12, 2025, 16:25 - 17:50

Stable phase-change materials are of great significance for relieving the contradiction of energy supply and demand. On this front, nano-enabled phase change materials (PCMs) are gaining significant attention for cold storage and transportation due to their enhanced thermal properties, stability, and energy efficiency. This study explores the development of a stable emulsion of nano-enabled PCMs for cold chain applications, where maintaining precise temperature control is essential for perishable goods such as food, pharmaceuticals, and biological samples. By incorporating nanoparticles—such as metal oxides (TiO2, SiO2, Al2O3), carbon-based materials (CNTs, Graphene, and Mxenes—into traditional PCMs, the thermal conductivity and latent heat capacity are improved, leading to faster charging/discharging cycles and more reliable cooling. However, challenges like phase separation, leakage, and agglomeration in emulsions must be addressed to ensure long-term stability. This research focuses on stabilizing nano-PCMs in emulsions using surfactants and advanced encapsulation techniques, achieving enhanced durability under repeated thermal cycling. Experimental results demonstrate the potential of these materials to maintain low temperatures with reduced energy consumption during transport, improving efficiency in cold chain logistics. The findings suggest that nano-enabled PCM emulsions offer a promising solution for sustainable and reliable cold storage systems.

Thermoacoustic characterization of phase change materials

Dr Laura A. Cobus[1], Fouzia Achchaq[2]
[1]University Of Canterbury, Christchurch, New Zealand, [2]University of Bordeaux, Talence, France

Session 9A: Thermal management and materials, Auditorium, February 12, 2025, 16:25 - 17:50

To mitigate climate change, sustainable energy generation and management is crucial. Heat poses a particular problem; while roughly 90% of global energy use involves the generation or manipulation of thermal energy [1], around 50% of that will be wasted [2]. To better capture, store, and control thermal energy, specialized heat storage materials can be used, with the best heat storage density offered by phase change materials (PCMs) due to the latent heat they release/absorb when undergoing a phase change. Among many potential applications, PCMs could vastly improve the exploitability of renewable energy sources [3].

To evaluate the potential of new PCMs, and to monitor their behaviour in industrial settings, it is critical to understand their chemical, thermal, and mechanical properties. In this talk, we will discuss the characterization of a new lithium-hydroxide-based PCM [4] recently created at the University of Bordeaux. By integrating acoustic, thermal, and microscopic imaging/characterization techniques, very surprising and potentially useful material properties were found for the solid phase of this PCM.

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Momentum for catalysis: how surface reactions shape the RuO2 flat surface state

Dr Vedran Jovic[1], Mr Christopher Reiser[2], Mr Philipp Keßler[2], Dr Martin Kamp[2], Dr Simon Moser[2]
[1]Earth Resources and Materials, Institute of Geological and Nuclear Science, Lower Hutt, New Zealand,
[2]Physikalisches Institut, Universität Würzburg, Würzburg D-97074, Germany

Session 9B: Synchrotron-based methods for materials science and engineering, Dobson 1,
February 12, 2025, 16:25 - 17:50

Utilising state-of-the art synchrotron spectroscopy, we present the first simultaneous in operando and momentum resolved study of hallmark surface chemical reactions on the benchmark oxygen evolution (hydrogen production) catalyst RuO2. We exploit the site selectivity of these surface chemical reactions to experimentally characterize the microscopic electronic properties of RuO2's Dirac nodal lines and flat band surface state – answering pertinent questions on its topology by means of applied surface chemistry. Our results underline two important aspects: First, the modification of an ordered catalyst's surface band structure through site selective surface reaction can be used to monitor catalytic process in operando, with momentum as an additional source of information beyond what conventional XPS can deliver. Second, but more importantly, the delocalized surface electronic band structure, i.e. momentum governed Bloch states, were shown to actively participate in the reaction process. Tapping into this resource sheds new light on traditional tenets of surface chemistry, such as the fully local Blyholder picture, and offers a means to bridge the gap between solid-state physics, surface chemistry and catalysis.

Understanding anomalous cyclic voltammetric behaviour of gold clusters

Dr Shailendra Kumar Sharma[1], Prof. Aaron Marshall[1]
[1]University of Canterbury, Christchurch, New Zealand

Session 9B: Synchrotron-based methods for materials science and engineering, Dobson 1, February 12, 2025, 16:25 - 17:50

An industry-scale implementation of electrocatalysis is one of the most promising ways to enable the sustainable production of valuable chemicals and to reduce the dependence on fossil fuels. Metal clusters have attracted vivid interest in catalysis due to strong size- and composition-dependent catalytic performance. Nanoclusters are sub-2 nm nanoparticles with atomically precise chemical composition and structure. They are made of a core of metal atoms bonded together and capped with the organic periphery, preventing their agglomeration in the solution phase [1, 2].

Surprisingly, even though the clusters possess a majority of Au atoms on the surface, Au oxide reduction behaviour is not generally observed in their cyclic voltammetry [3, 4]. This suggests that either the Au clusters show different oxidation/reduction behaviour cf. the bulk or the metal/electrolyte interfacial area is considerably lower due to passivation of the surface in the presence of capping ligands [5].

Here, we studied cyclic voltammetry of a series of atomically precise Au clusters. We observed that while the as-made electrode fails to show Au/AuOx reduction behaviour during repeated cycling CVs change significantly after electrolysis, and the Au/AuOx peak becomes visible. Interestingly, the growth of the peak was dependent on the nature of the ligand and the nuclearity of the clusters. We used in-situ X-ray absorption spectroscopy to study the structural evolution of cluster-based catalysts to understand their anomalous cyclic voltammetric behaviour. A detailed discussion on the experimental design, and the analysis of electrochemical, X-ray absorption studies and challenges will be given in the conference contribution.

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Advanced Nanocellulose composites for Information processing

Dr. Elena Bencurova[1], Aman Akash[1], Professor Thomas Dandekar[1]
[1]University of Würzburg, Germany, Würzburg, Germany

Session 9C: Biosensors, Dobson 2, February 12, 2025, 16:25 - 17:50

In my talk I will discuss the attractive features of nanocellulose for better information processing: This includes light-gated enzymes which then synthesize DNA according to light-signals and modify a DNA storage including its read-out. The DNA is particularly well protected in the nanocellulose composite. Latest data and designs will explain and show how the light-gated enzymes can be improved and designed in such a DNA storage operation task as well as alternative applications.

We will also explain latest developments on nanocellulose itself, in particular its potential for full nanocellulose transistors and different extensions of the nanocellulose compound relevant for optimal information processing in this device, the nanocellulose chip.

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Electrical characterization of thin films for carbon nanotubes for gas phase biosensor applications

Mr Sangar Begzaad, Dr Gideon Gouws, Dr Natalie Plank
[1]Victoria University of Wellington, Wellington, New Zealand, [2]Victoria University of Wellington, Wellington, New Zealand, [3]Victoria University of Wellington, Wellington, New Zealand

Session 9C: Biosensors, Dobson 2, February 12, 2025, 16:25 - 17:50

Single-walled carbon nanotubes (CNTs) can be either metallic or semiconducting depending on how the material has been formed during synthesis [1]. Thin films of carbon nanotubes are a useful functional platform for biosensors, either in the liquid or gas phase [2,3]. Adsorption or binding of molecules onto the surface of the CNTs induces changes in the charge distribution and electronic environment of the CNTs resulting in the change in conductivity of the CNTs films. Hence, one of the criteria for utilization in resistive gas phase sensing is the reliability of the electrical performance of the films [3,4]. In this study, we have fabricated thin films of carbon nanotubes using metallic and semiconducting films of known electrical purity from Nanointegris (iso-nanotube 90% semiconducting, and 90% metallic). The physical composition of the film has been controlled via a solution deposition method, where the number of rounds and the deposition times for the CNTs have been varied. The thin film morphology has been characterized using atomic force microscopy (AFM) and applying an automated statistical analysis method on the films. The electrical properties of the films have been investigated using Van der pauw (VDP) electrical measurement techniques, and the performance linked to the AFM morphology. We then investigate the utility of the CNT thin films as a gas-sensing platform.

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Comparative Analysis of Adenosine CNT-FET Aptasensor performance: Impact of Functionalization Routes and Buffer Solutions

Mr Alireza Zare[1,2], Miss Danica Fontein[1,2], Dr Natalie Plank[1,2]
[1]Victoria University of Wellington, Wellington, New Zealand, [2]The MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand

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Carbon Nanotube Field-Effect Transistors (CNT-FETs), well-known for their superior electronic properties[1], are used as the active layer of the biosensor platform[2]. The specific carbon chemistry of CNTs facilitates the attachment of biorecognition elements[3], enabling point-of-care detection of small target molecules down to picomolar concentrations in a liquid environment[4].

We employ an adenosine aptamer with the sequence of a 35-mer[5] as the biorecognition element on a liquid gated network CNTFET channel, achieving successful detection of adenosine at picomolar concentration level. To facilitate a comparative analysis of different functionalization routes and biological buffer solutions impact on device performance, multiple CNTFETs with similar electrical properties are fabricated, ensuring a consistent electronic platform.

In this study, 1-pyrenebutanoic acid succinimidyl ester (PBASE) is employed as a molecular linker to covalently immobilize the -NH2 functionalized aptamer receptor. The attachment to the carbon nanotube (CNT) walls is maintained noncovalently through π-π stacking interactions. To examine the robustness of CNT functionalization, Tris-HCl and Phosphate-Buffered Saline (PBS) are used as biological buffer solutions across various functionalization protocols. We will present a comparative analysis of the sensing capabilities of CNT-FET adenosine biosensors, focusing on their sensitivity, selectivity, reproducibility, and overall performance under different functionalization conditions.

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Smart and multifunctional chitosan film as a biosensor in intelligent food packaging

Mr Shuva Bhowmik[1,2], Dr Dominic Agyei[2], A/Prof. Azam Ali[1]
[1]Centre for Bioengineering and Nanomedicine, Faculty of Dentistry, Division of Health Sciences, University of Otago, Dunedin, New Zealand, [2]Department of Food Science, Division of Sciences, University of Otago, Dunedin, New Zealand

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Background: Microbial contamination is a typical occurrence during the storage of perishable foods, resulting in poor food quality and a risk to consumer health1. Perishable foods' short shelf life and insufficient packaging are expected to lead to a more than 200 million tonnes increase in food waste by 2050. As a result, the food industry may protect food by using multifunctional food packaging materials to prevent contamination, monitor food deterioration, reduce food waste, and ensure food safety2,3. Hence, this study explored sustainable resources, specifically marine chitosan and its derivative chitooligosaccharides (COS), bioactive colour-changing compounds, in the preparation of multifunctional smart film.

Methods: The aqueous conventional solvent casting technique was employed to fabricate the multifunctional smart film. The functional, physicochemicals, biodegradability, and cytotoxicity profile were examined.

Results: The incorporation of COS and other bio-additives in the chitosan film resulted in a notable improvement in the mechanical, barrier, and thermal properties of films. The release of bioactive compounds from the fabricated film significantly enhanced its antioxidant (97%) and antimicrobial activity (>50%) towards both Gram-positive and Gram-negative bacteria. Furthermore, the multifunctional chitosan films demonstrated a significant colour change from red to yellow in pH 1-14 and acted as a biosensor. Additionally, more than 80% cell viability was observed towards HaCaT cells, indicating their safe use for food packaging.

Conclusions: The research findings revealed that the fabricated smart and multifunctional marine biopolymer film could have potential in the applications of the intelligent food packaging industry to extend food shelf life and track food spoilage.

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Optimizing LAMP Assays for In-Field Detection of Kauri Dieback Pathogens

Ms Zhuoyue Wang[1], Prof Volker Nock[1], Dr Claudia Meisrimler[1]
[1]University Of Canterbury, Christchurch, New Zealand

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The rapid spread of kauri dieback, caused by Phytophthora agathidicida and Phytophthora cinnamomi, presents a significant threat to the New Zealand native kauri tree and ecosystems. The key to effective management is early and accurate detection of the spread of the disease. Loop-mediated isothermal amplification (LAMP) offers a promising solution due to its suitability for rapid in-field detection that is facilitated by its isothermal nature and minimal equipment requirements. Recent studies have shown the potential of LAMP assays in detecting Phytophthora species [1,2].

However, current LMAP assays are complicated by false positive and inconsistent amplification results [3]. This study aims to improve the reliability of the existing LAMP assays for future integration into capillaric microfluidic devices for in-field detection [4,5]. The primer design process was carefully refined through iterative testing to ensure high specificity and efficiency in amplifying the target sequences. The LAMP assay was further optimized by testing various additives to enhance specificity and minimize false positives. Additionally, dyes that are commonly used in LAMP detection were compared to determine their impact on result clarity and reliability.

The results of this comparative study will enhance plant pathogen detection, ensuring quick and accurate responses in various conditions, thus providing a strong foundation for the future development of reliable in-field diagnostic microfluidic devices. These advancements are crucial for the early detection and management of kauri dieback, helping to protect New Zealand’s iconic kauri tree from this devastating disease.

Keyword: kauri dieback, Phytophthora species, LAMP, plant pathogen detection, microfluidics

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Enhancing the Performance and Longevity of Biomass Combustors: Leveraging Microtextures to Reduce Soot Accumulation

Oz Oren[1], Gordon McTaggart-Cowan[1], Dr Sami Khan[1]
[1]Simon Fraser University, Surrey, Canada

Session 9D: Textured surfaces, Dobson 3, February 12, 2025, 16:25 - 17:50

Biomass combustion provides daily energy and food needs for millions of people worldwide [1]. However, soot accumulation on the walls of the combustors is a challenge. Soot accumulation can increase thermal resistance, thereby impeding heat transfer from the combustion process to the surroundings [2].

Herein, we demonstrate a novel approach to reduce soot accumulation on surfaces using microtextures. We investigate soot layers from the combustion of paraffin oil as a model for wood-based soot. A custom setup was designed to deposit soot uniformly, and we selected glass as the substrate of interest to investigate soot oxidation. We observe that randomly microtextured glass obtained by sandblasting shows a 71% reduction in the time taken to oxidize 90% of surface soot coverage when compared to smooth glass at 530°C. Using optical microscopy, we find that the oxidation initiated on the sharp peaks within the sandblasted surface and then propagated radially around each peak until the propagation fronts from neighbouring peaks merge. Analysis by X-ray Photoelectron Spectroscopy (XPS) validates the superior extent of soot removal on microtextures down to a sub-nanometer length-scale. We also study grooved microtextures fabricated via laser ablation and find that grooves with widths between 15 and 50 µm enhance soot oxidation, while the expedited advantage is lost when the groove width is 85 µm, indicating that there is an optimal length-scale of surface roughness for this self-cleaning effect to take place.

Microtextured surfaces that facilitate soot oxidation upon contact could significantly improve performance and longevity in various combustion applications.

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Femtosecond Laser Processing and Other Methods to Create Micropatterned Surfaces for Energy Applications

Dr Kirill Misiiuk[1,2,3], Prof. Richard Blaikie[1,2,3], Dr Sam Lowrey[1,2,3]
[1]University of Otago, Dunedin, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, Dunedin, New Zealand, [3]Dodd-Walls Centre for Photonic and Quantum Technologies, Dunedin, New Zealand

Session 9D: Textured surfaces, Dobson 3, February 12, 2025, 16:25 - 17:50

Energy technologies always demand cutting-edge, novel solutions to increase the efficiency of any process. Interaction of a liquid with a solid surface is a problem that unites many energy applications: condensation on plates of heat exchangers, droplet erosion of blades of steam turbines, condensation and freezing on blades of wind turbines and aircraft, etc. For industrial applications it is required to have durable and easy casting materials, thus everything is made of metals or at least has a metallic coverage. This brings a set of challenges due to their relatively high adhesive forces.

Accepting the challenge and looking back at the examples in nature, topographical modifications of various solid materials, especially metals, were investigated by our team. A few solutions could be proposed to make coating-less surfaces with various wetting characteristics. Such surfaces could be made via one-step industrial methods - Femtosecond Laser Processing, in a very controllable way and fulfil certain purposes like passive manipulation of micro-scale water droplets to impact the condensational behaviour.

Starting from the open surface and a simple deposition of water droplets, we have expanded our knowledge by investigating various substrates, and nuances of the manufacturing and analytic tools to create and test the manufactured microstructures. We will present current results, discuss their potential for energy applications and cover new avenues for manufacturing opportunities.

Unveiling Structure Selectivity Relationships in Electrochemical CO2 Reduction Using Patterned Electrodes

Mr Campbell Tiffin[1,2], Dr. Kirill Misiiuk[2,3], Dr. Sam Lowrey[3,4], Dr. Sami Khan[5], Professor Aaron Marshall[1,2]
[1]Department of Chemical and Process Engineering, University of Canterbury, Christchurch, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, New Zealand, [3]Department of Physics, University of Otago, Dunedin, New Zealand, [4]Dodd-Walls Centre for Photonic and Quantum Technologies, New Zealand, [5]School of Sustainable Energy Engineering, Simon Fraser University, Surrey, Canada

Session 9D: Textured surfaces, Dobson 3, February 12, 2025, 16:25 - 17:50

As global carbon dioxide (CO_2) emissions continue to grow uncontrollably, the need for processes to capture and convert CO_2 is exacerbated. CO_2 can be converted into a range of useful value-added chemicals and fuels, such as methane (CH_4), the main component of natural gas and ethylene (C_2H_4), a key precursor in the production of polyethylene, the most commonly used plastic, through the electrochemical CO_2 reduction reaction (ECO_2RR) and by utilising renewable energy sources such as solar, wind and hydro, to power the reaction, there are no net emissions and a carbon-neutral fuels and chemical cycle can be achieved.[1] Despite extensive study since the 1980s, ECO_2RR's performance (selectivity and activity) still limits its commercialisation. Several factors influence its performance, including electrode material[2], crystal facet[3], morphology[4], electrolyte and its concentration[5] [6], local and bulk pH[7] [8], and mass transfer[9] [10]. Electrode structuring is a common method for controlling the local electrode environment and steering the reactions selectivity. However, these structures typically consist of tortuous, ill-defined nanostructures, making it challenging to understand the impact of different morphological features (e.g., roughness and porosity) on ECO_2RR performance.

In our research, we employ surface laser texturing to create electrodes with periodically patterned arrays of microchannels, pillars, pores, and pyramids. We compare the performance of these electrodes by varying the feature size and spacing of each pattern. By studying periodically patterned arrays, we gain insights into optimizing electrodes for the commercialisation of ECO_2RR.

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Fabrication of Nano- and Microstructures on Polysulfides Surfaces

Miss Abigail Mann[1,2], Dr Lynn Lisboa[1,2], Mr Samuel Tonkin[1,2], Dr Pankaj Sharma[1,2], Dr Jason Gascooke[2,5], Dr Christopher Gibson[3,4], Professor Justin Chalker[1,2]

[1]Institute for Nanoscale Science and Technology, College of Science and Engineering, Flinders University, Bedford Park, Australia, [2]College of Science and Engineering, Flinders University, Bedford Park, Australia, [3]Flinders Microscopy and Microanalysis, College of Science and Engineering, Flinders University, Bedford Park, Australia, [4]Adelaide Microscopy, The University of Adelaide, Adelaide, Australia, [5]Australian National Fabrication Facility, South Australia Node, College of Science and Engineering, Flinders University, Bedford Park, Australia

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Sulfur-based polymers are rapidly gaining interest in applications such as infrared optics, metal remediation and energy storage .[1, 2] These polymers, when made from sulfur and either dicyclopentadiene or cyclopentadiene,[3, 4] exhibit glassy black surfaces with roughness below 1 nm, offering a new avenue for a range of applications. Two methods for modifying the surface of these polymer will be presented. The first method utilises a low-power laser (~1-5 mW) for fabricating microscale structures on the surface via a novel and direct lithographic process.[5] This energy-efficient and robust technique enables fabrication of microscale structures with applications in optics, data storage, microfluidics, and surface engineering. The second application involves using nanoscale indentation using probe-based systems, offering control of depth of the indentations. These features can be used to store information on the polymer using binary or ternary and other encoding systems, making it promising for high-density, re-writable data storage applications [6]. These studies advance micro and nano-scale surface engineering to expand the range of applications of sulfur-based materials.

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Stochastic Spiking in Percolating Networks of Nanoparticles enables Optimization and Classification

Miss Sofie Studholme[1,2], Dr Zac Heywood[1,2], Dr Josh Mallinson[1,2], Dr Simon Brown[1,2]
[1]University Of Canterbury, Christchurch, New Zealand, [2]The MacDiarmid Institute for Advanced Materials and Nanotechnology, Christchurch, New Zealand

Session 9E: Neuromorphic unconventional and physical computing Symposium, Dobson 4, February 12, 2025, 16:25 - 17:55

Self-assembled Percolating Networks of Nanoparticles (PNNs) are of interest for neuromorphic computing due to their brain-like properties, CMOS compatibility and potential for ultra-low power consumption. PNNs are fabricated by depositing conducting nanoparticles onto a substrate until the percolation threshold is reached. At this point, the network architecture is brain-like as it is small-world and scale-free. Atomic scale spiking dynamics in PNNs meets criticality criteria, which is associated with optimal computation and thought to be the operating point of biological brains [1,2]. Here we investigate how spiking PNNs can be exploited for neuromorphic computing. First, we employ a rate coding scheme in which binary patterns, encoded as voltage levels, are applied to the PNN and the event rate is used to perform logical operations and image classification [3]. We then show spiking can be used in a probabilistic computing scheme. Using an algorithm inspired by adiabatic quantum computing [4], factorization of integers is demonstrated. These preliminary results show exciting potential for exploiting spiking PNNs to solve complex optimisation problems.

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The growth and stability of nanofilaments in atomic switches

Dr Kannan Ridings[1,2]
[1]The University of Auckland, Auckland, New Zealand, [2]The MacDiarmid Institute of Advanced Materials and Nanotechnology, Auckland, New Zealand

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Atomic switches (AS) and atomic switch networks (ASN) are promising technologies for next-generation computing, offering a pathway to replace conventional transistor-based systems [1-3]. These devices operate by the formation and dissolution of atomic-scale conductive filaments (CFs), enabling high-density, low-power switching. However, challenges related to the stability of these filaments, particularly due to Joule heating, and the reliability of their growth and shrinkage, need to be addressed for practical implementation [4,5].

In this research, I employ molecular dynamics simulations to explore the stability and growth mechanisms of CFs in ASNs [6, 7]. By investigating various material systems and parameter spaces, I aim to identify strategies for enhancing CF stability and optimizing the performance of AS devices. This work seeks to provide critical insights into the behavior of nanofilaments in ASNs, contributing to the development of robust, energy-efficient computing technologies.

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Modeling and theoretical insights into capacitive, inertial, and resistive effects in memristive devices for neuromorphic systems

Dr Sahitya Yarragolla[1], Mr Torben Hemke[2], Dr Tobias Gergs[1], Dr Jan Trieshchmann[1], Dr Thomas Mussenbrock[2]
[1]Theoretical Electrical Engineering, Faculty of Engineering, Kiel University, Kiel, Germany, [2]Chair of Applied Electrodynamics and Plasma Technology, Ruhr University Bochum, Bochum, Germany

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This work examines the coexistence of resistive (R), capacitive (C), and inertia (virtual inductive, L) effects in memristive devices, with a particular emphasis on their implications for the field of neuromorphic computing. Recent studies have demonstrated that these RLC effects exert a significant influence on technical analog of synaptic activities, including short- and long-term plasticity, which are of paramount importance for the replication of the intricate dynamics observed in biological synapses [1]. These effects have been observed across a range of memristive devices, including nanowire networks, nanoparticle networks, and resistive switching devices, all of which are considered key candidates for use in neuromorphic systems. Therefore, our work is based on the necessity to develop a comprehensive theoretical framework that delves into the underlying physical and chemical processes contributing to the diverse switching behaviors observed in these devices establishing a robust foundation for practical applications in neuromorphic computing. For this, physics-inspired compact model and multi-dimensional models for resistive switching devices [2] and nanoparticle networks [3,4] are refined to integrate capacitive and inertial effects, thereby offering more realistic and precise predictions of dynamic current-voltage and capacitance-voltage characteristics [5,6]. These predictions thereby provide valuable insights for optimizing device performance in neuromorphic systems. It is of paramount importance to comprehend frequency-dependent nonlinearity of these devices, as RLC effects are subject to variation with input frequency, exerting a considerable influence on the device's behavior. This work contributes to our comprehension of these multifaceted effects, facilitating the development of more effective and reliable neuromorphic hardware.

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Temperature regulation as instance of homestasis with bio-inspired feedback mechanisms

Miss Maximiliane Noll[1], Petro Feketa[2], Tom Birkoben[1], Alexander Schaum[3], Thomas Meurer[4], Hermann Kohlstedt[1,5]

[1]Chair for Nanoelectronics, Kiel University, Kiel, Germany, [2]School of Mathematics and Statistics, Victoria University of Wellington, New Zealand, [3]Chair for Process Analytics, University Hohenheim, Stuttgart, Germany, [4]Digital Process Engineering Group, Institute for Mechanical Process Eng. and Mechanics, Karlsruhe Institute of Technology, Karlsruhe, Germany, [5]Kiel NanoSurface and Interface Science KiNSIS, Kiel University, Kiel, Germany

Session 9E: Neuromorphic unconventional and physical computing Symposium, Dobson 4,
February 12, 2025, 16:25 - 17:55

To maintain robust functioning, the concept of homeostasis, introduced by Cannon [1], enables living organisms to adapt to changing environments [2]. A common example of homeostatic behavior is the stable internal temperature of mammals [3]. In this work, we present an electronic implementation of temperature regulation based on a single-effector regulation system. The foundation of the electronic circuit consists of two thermosensitive neurons equipped with temperature dependent resistors. Their spikes are processed by a summation unit, with the output fed back through a feedback loop that causes a Peltier element to heat or cool a metal plate. On top of the metal plate the temperature dependent resistors of both neurons are placed and are therefore influenced by the Peltier elements temperature. By processing the spike trains, an inherently unknown system set-point can be stabilized. We examine key parameters, including the influence of feedback control gain and the activity patterns of the thermosensitive neurons on the set-point. While neuronal interconnections are not strictly necessary for stabilizing the set-point, we hypothesize that synaptic plasticity in mammals may represent an additional control layer that enhances system robustness. [4]

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Glasses made from hybrid perovskites and metal-organic frameworks: Characterisation and Properties

Thomas Bennett[1]
[1]University of Canterbury, Christchurch, New Zealand

Plenary Session 5, Auditorium, February 13, 2025, 08:30 - 09:30

Porous frameworks are heavily promoted for use in catalysis, gas separations, water harvesting and drug delivery. On the other hand, more dense materials, hybrid organic-inorganic perovskites, are proposed as next generation photovoltaic and barocaloric materials. In both cases, order—or uniformity— is frequently held to be advantageous, or even pivotal, to our ability to engineer useful properties in a rational way.

Disordered materials, such as glasses, are however ubiquitous in our daily lives. Inorganics for example open our eyes to the world (through lenses and display screens), provide housing materials and warmth, and allow us to retrieve not only energy, but also digital memories. Organic glasses protect our health through antimicrobial coatings and shatter-proof screens, and metallic glasses promise surgical tools for life-saving interventions.

This talk covers the gap between these two fields, and considers the formation of hybrid glasses. Such glasses contain linked organic and inorganic components, and thus are now considered to belong to a 4th category of glass chemistry. This talk highlights their formation, structural characterisation, and promise in application.

Looking into the future of hybrid glasses
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Mechanochemically-induced glass formation from two-dimensional hybrid organic–inorganic perovskites
C. Ye, G. I Lampronti, L. N McHugh, C. Castillo-Blas, A. Kono, C. Chen, G. P Robertson, L. Nagle-Cocco, W. Xu, S. D Stranks, V. Martinez, I. Brekalo, B. Karadeniz, K. Užarević, W. Xue, P. Kolodzeiski, C. Das, P. Chater, D. A Keen, S. E Dutton, T. D Bennett*, Chem. Sci., 2024, 15, 7198-7205.
Liquid metal-organic frameworks.
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Soft Materials to Understand Cell-Material Interactions and to Pattern Magnetic Clusters

A/Prof Jenny Malmstrom[1,2], Dr Anaïs E Chalard[1,2], Mr Harrison Porritt[1,2], Dr Annika Winbo[3], Dr Daniel Clyde[1,2,4], Professor Juliette Fitremann[5], Professor Andrew Taberner[6], Dr Alex Dixon[6], Professor Penelope Brothers[7], Dr David Cortie[8], Dr Simon Granville[2,9]
[1]Chemical and Materials Engineering, University of Auckland, Auckland, New Zealand, [2]The MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand, [3]Department of Physiology, The University of Auckland, Auckland, New Zealand, [4]School of Chemical Sciences, University of Auckland, Auckland, New Zealand, [5]Laboratoire Softmat, Université de Toulouse, Toulouse, France, [6]The Auckland Bioengineering Institute (ABI), The University of Auckland, Auckland, New Zealand, [7]Research School of Chemistry, Australian National University, Canberra, Australia, [8]Australian Nuclear Science and Technology Organisation, Lucas Heights, Australia, [9]Robinson Research Institute, Victoria University of Wellington, Wellington, New Zealand

Keynote Session 15, Auditorium, February 13, 2025, 09:35 - 10:10

In our research group, we use materials engineering to understand biology better, and to create advanced materials. This talk will cover topics from self-assembly to pattern polyoxometalates (POMs) at surfaces to how we engineer hydrogels to better understand how mammalian cells sense their surroundings. These topics are linked by the materials engineering approaches used but highlight two very different applications of soft materials.

Our hydrogel research stems from a need for better experimental systems to understand how mammalian cells sense and adapt to mechanical cues from their microenvironment. We have developed a projection method to spatially photopattern the mechanical properties of Gelatin methacrylol (GelMA) hydrogels [1] and we have combined the GelMA with biocompatible supramolecular fibers made of a small self-assembling sugar-derived molecule (N-heptyl-D-galactonamide, GalC7). The GalC7 fibrous network was found to increase the Young's modulus of GelMA and observed to dissolve over time, leading to a dynamic softening of the composite gels. [2]

Self-assembly is also a crucial tool in our patterning work where we use a block copolymer-assisted strategy to pattern arrays of POMs on silicon and permalloy substrates. We have investigated the magnetic properties of these materials and, interestingly, the data show that a thin layer of patterned POMs strongly influenced an underlying permalloy layer. This work demonstrates that the bottom-up pathway is a potentially viable method for patterning magnetic substrates on a sub-100 nm scale, toward the magnetic nanostructures needed for spintronic or magnonic crystal devices. [3]

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Unveiling the hidden secrets of spintronic materials with neutron scattering

Professor Kirrily Rule[1,2]
[1]ANSTO, Lucas Heights, Australia, [2]University of Wollongong, Wollongong, Australia

Keynote Session 16, Dobson 1, February 13, 2025, 09:35 - 10:10

Neutron scattering is a powerful tool for investigating magnetic materials due to the neutron's intrinsic quantum spin value S=1/2. We use neutrons to search for materials that could revolutionise computing technology via the field of spintronics. Spintronics exploits the intrinsic spin of electrons, and fundamental to this field is controlling the flows of the spin degree of freedom, i.e., through spin currents. Much of the foundational knowledge in this field was made possible by fundamental discoveries that were recognized by the 2016 Nobel Prize in Physics.

I will give details of different neutron scattering techniques which can be used to probe the spin-properties of potential spintronics materials. This keynote talk will include examples using polarised neutron techniques [1], time of flight inelastic neutron scattering [2,3], and others [4].

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Designing Metal Single Atom Catalysts for Tomorrow’s Energy Sector

Professor Geoffrey Waterhouse[1,2]
[1]The University Of Auckland, Auckland, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, New Zealand

Session 10A: Catalysis and Innovative materials, Auditorium, February 13, 2025, 10:40 - 12:45

Metal single-atom catalysts (SACs) are increasingly being utilized in electrocatalysis and thermal catalysis owing to their (i) fully exposed active sites, (ii) very high metal atom utilization efficiencies, and (iii) tunable local coordination geometries which allows modulation of both activity and selectivity for particular applications. This lecture will overview some of my group’s recent collaborative research aimed at the design of durable SACs for various selective chemical transformations linked to the renewable energy sector, including the oxygen evolution and reduction reactions (OER/ORR), hydrogen evolution and oxidation reactions (HER/HOR), and carbon dioxide conversion to fuels. By judicious selection of both metal and underlying support, efficient and durable SACs for all these processes can be realized. Challenges relating to the design of metal SACs for energy storage/conversion will be discussed, specifically how high metal loadings can be achieved without undesirable metal nanoparticle formation. A newly discovered universal route synthetic towards ultra-high-density M-N-C SACs (with loadings >20 wt.% for many metals) will be introduced, paving the way for the widespread commercial adoption of SACs across the energy sector (e.g. use in rechargeable zinc-air batteries, PEMFCs and the production of sustainable aviation fuels).

Are Transition Metal (Oxy)Nitrides Active Catalysts for Electrochemical Nitrogen Reduction?

Dr Prasanth Gupta Sridhar Gupta[1,2], Mr Zulfitri Rosli[1,2,3], Dr Siriluck Tesana[1], Dr Niall Malone[1], Dr John Kennedy[1,2]

[1]National Isotope Centre, GNS Science, Lower Hutt, New Zealand, [2]The MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, Wellington, New Zealand, [3]Faculty of Chemical and Materials Engineering, The University of Auckland, Auckland, New Zealand

Session 10A: Catalysis and Innovative materials, Auditorium, February 13, 2025, 10:40 - 12:45

The direct electrochemical nitrogen reduction reaction (eNRR) presents a promising pathway to produce ammonia for green fertilizers and as zero-carbon energy vectors. Despite extensive research, an active catalyst capable of performing eNRR in aqueous electrolytes under ambient conditions remains elusive [1,2]. Certain transition metal nitrides (VN, ZrN, NbN) are theoretically predicted to facilitate eNRR via the Mars-van Krevelen mechanism, but experimental validation is lacking.

In this study, we explore the ability of ion-beam synthesized transition metal (oxy)nitride (TMON) thin film catalysts to perform eNRR via the Mars-van Krevelen mechanism. Ion beam synthesis offers a non-thermal equilibrium pathway to access metastable and high-temperature phases with enhanced catalytic activity [3-5]. We report the fabrication of TMON catalysts through low-energy nitrogen implantation into vanadium and zirconium thin films, which were produced via ion beam sputtering. Comprehensive characterization of surface composition, structure, topography, and chemical bonding was conducted using ion beam analysis, X-ray diffraction, high-resolution transmission electron microscopy, atomic force microscopy and X-ray photoelectron spectroscopy.

To ensure accurate measurement of electrochemically produced ammonia, we employed stringent and rigorous eNRR protocols to distinguish it from ubiquitous contamination. These protocols are briefly outlined, and the electrochemical performance of the TMON catalysts (Faradaic efficiency and production rates) are reported. We compare the electrochemical performance from our study with existing literature, highlighting novel pathways for future research advancements.

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Stable organic cages from aromatic macrocycles: inclusion and assembly

Professor Nigel Lucas[1], Dr Courtney Ennis[1], Jona Fischer[1], Dr Ramkrishna Mandal[1]
[1]University of Otago & MacDiarmid Institute for Advanced Materials and Nanotechnology, Dunedin, New Zealand

Session 10A: Catalysis and Innovative materials, Auditorium, February 13, 2025, 10:40 - 12:45

Confined spaces within self-assembled capsules and molecular cages are distinct from the bulk solvent, sequestering complementary guests or catalysing chemical reactions.[1] While hydrogen-bonded assemblies of other molecular bowls are known, the majority of reported capsules are built upon the readily available resorcin[4]arene macrocycle scaffold, the intrinsic concave surface and an exoannular array of hydroxyl groups providing the elements for capsular self-assembly.

We have reported[2] the synthesis of a novel resorcin[4]arene-derived octamethoxy cavitand with an enforced, conical cavity. The related octol has been investigated for self-assembly behaviour in solution in a range of solvents.[3] NMR experiments show the cavitand readily dimerizes through a seam of interdigitated hydrogen-bonds The well-defined cavity preferentially encapsulates small cationic guests, replacing the guest solvent.

The propensity for organic cations to interact strongly with this aromatic-rich cavitand prompted us to investigate the cation-templated synthesis of covalent organic cages from related resorcin[4]arene building blocks. Chiral cages are formed exclusively from a mixture of cavitand reactants in the presence of a cation that, depending of the cage size, remains mechanically included or can be exchanged for solvent.

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Growth of a Poyoxometalate-Capped Giant Iron-Based Molecular Mineral Structure from Water

Dr Masooma Ibrahim[1]
[1]Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Session 10A: Catalysis and Innovative materials, Auditorium, February 13, 2025, 10:40 - 12:45

Recently, the discovery of naturally occurring polyoxometalates (POMs) in mineral structures demonstrates their importance in geochemical systems [1,2]. Understanding and identifying the hydrolysis products of iron in aqueous systems is crucial for comprehending the formation of iron minerals. Using a “bottom-up” approach, a giant iron-based molecular mineral $\{Fe_{32}O_{45}Na_6(OH_2)_{18}\}^{12+}$ (1.7 nm × 1.0 nm) has been synthesized from water in the presence of a suitable inorganic ligand through the controlled hydrolysis of iron salts. The oxidatively robust POM ligand $[P_2W_{15}O_{56}]^{12-}$ not only stabilizes and crystallizes the iron-oxo cluster but also imparts its intrinsic properties, such as solubility, stability, and electron trapping capability, to the isolated product $[Fe_{32}O_{45}Na_6(OH_2)_{18}(P_2W_{15}O_{56})_6]^{60-}$. The reduction of 32 Fe^{3+} centers to Fe^{2+} while retaining structural integrity makes this system promising for electrocatalytic reduction processes. Our synthetic approach may provide a molecular pathway for geochemical reactions during the mineralization process.

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Textile Sensor Consists of 2D Materials

Prof Azam Ali[1], Dr. Nazmul Islam[2], Dr. Stewart Collie[3]
[1]Otago University, Dunedin, New Zealand, [2]Centre for Bioengineering & Nanomedicine, University of Otago, Dunedin, New Zealand, [3]Bioproduct & Fibre Technology, AgResearch, Christchurch, New Zealand

Session 10A: Catalysis and Innovative materials, Auditorium, February 13, 2025, 10:40 - 12:45

Wearable e-textiles based on carbon materials have provided the impetus for the academic and industrial sectors to analyse the physical performance of a sportsman or heartbeat, the health record and follow-up in real time of patients and personal protective equipment. Since the debut of embedded circuits into textile or clothing, one question that is consistently asked by researchers is “Can I wash it?” An innovative approach was designed and applied to construct textile sensors from carbon nanotube (1D) and graphene (2D) in our research, and the study findings related to its durability and robustness against harsh environments in detail will be presented. The challenges for carbon materials (1D/2D) based conductive textile’s wash durability, bending, and flexibility will also be highlighted in my presentation. It’s recognized that large numbers of research are focused on wearable textile sensors, but the essential factors related to wear, care and sustainability aspects are often ignored. Nevertheless, different fabrication methods such as coating, screen printing, melt spinning, and encapsulation were applied to produce textile sensor in our research. The characterization of textile sensors consisting of graphene (2D) has been evaluated to assess the increase efficacy of sensors, as wearable technology.

Highly Active Catalysis by Ligand-promoted Stable, Low Loading, and High Dispersion of Pd

Mr Varinder Singh[1,3], Harry Cahyanto[2, 3], Alex C. K. Yip[2, 3], Professor Sally Brooker[1,3]
[1]Department of Chemistry, University Of Otago, Dunedin, New Zealand, [2]Department of Chemical and Process Engineering, University of Canterbury, Christchurch, New Zealand, [3]MacDiarmid Institute for Advanced Materials and Nanotechnology, New Zealand

Session 10A: Catalysis and Innovative materials, Auditorium, February 13, 2025, 10:40 - 12:45

Deactivation of metal nanoparticle catalysts due to agglomeration or sintering is a key issue in industrial catalytic chemical processes. Therefore, development of robust catalysts to increase the efficiency and durability of these catalysts is critical.1 Previously we demonstrated that L-histidine coordination to palladium (II) ions resulted in a uniform dispersion of Pd nanoparticles on fumed silica, maintaining high catalytic activity with low Pd-loading and extending catalyst life.2 Herein, similar results were achieved using ethylenediamine (EN) as a cheap bidentate ligand for in situ complexation of Pd(II) ions in water, which promotes the stable impregnation and dispersion of small Pd nanoparticles on a fumed silica catalyst support. Decomposition of EN at 225 °C in air for 48 hours yielded highly dispersed Pd(II) nanoparticles. Much higher dispersion was achieved for samples with high EN ratios. The dispersion was measured after hydrogen reduction using CO pulse chemisorption. After hydrogen reduction, these nanoparticles showed excellent catalytic activity and stability during propylene hydrogenation at 250 °C. An enhancement in catalytic activity was observed with increasing EN ratio for Pd:0EN to Pd:4EN, but similar high activity was observed for samples Pd:4EN to Pd:6EN. Also, on decreasing the catalyst loading (high space velocity) high catalytic conversion of propylene to propane sustained. Thus, a stable catalyst using cheap starting material with low Pd loading was achieved.

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Water and Light: Breaking Down Biofilms with Greener Photodynamic Materials

Professor Heather Buckley[1]
[1]University Of Victoria, Victoria, Canada

Session 10B: Materials for Environmental and Water Management, Dobson 1, February 13, 2025, 10:40 - 12:45

Unwanted microbial growth, and the chemistries used to address it, are a major source of persistent hazardous pollutants that impact both water security and ecosystem health. This and other challenges that limit availability of clean, safe abundant water for drinking and sanitation happen throughout the water cycle, and are amplified by social and environmental justice inequalities. These need to be addressed at a systems level that includes not only appropriate water treatment technologies, but also decisions about what materials are permitted to enter our waterways.

As green chemists and engineers, we have access to many tools through which we can contribute to sustainable water solutions and biofouling prevention. While technology is only one piece of the puzzle, we can use these tools to minimize the introduction of hazardous chemistries and materials in our waterways while still achieving the goal of safe drinking water for all.

This session will focus on green chemistry-inspired methods of targeting unwanted microbial growth, using covalent tethering of active molecules onto surfaces. Visible light in-situ production of short-lived reactive oxygen species offers effective prevention and removal of biofilms without the common hazardous chemical residuals of disinfection. This research combines small molecule synthetic chemistry, surface functionalization, photochemistry, diverse spectroscopies, and microbiological assays to provide a promising new class of antimicrobial materials.

Advanced Water Management Through Thermoresponsive Hydrogel Composites

Professor Jonghwi Lee[1]
[1]Chung-ang University, Seoul, South Korea

Session 10B: Materials for Environmental and Water Management, Dobson 1, February 13, 2025, 10:40 - 12:45

The urgent necessity for efficient and eco-conscious water management underscores a pivotal challenge in contemporary society. This study presents a groundbreaking approach by harnessing thermo-responsive hydrogels to drive water propulsion mechanisms, utilizing diurnal temperature variations. By embedding silicone into dehydrated hydrogel foams, we create a novel composite matrix. These porous hydrogels are engineered through a method of directional melt crystallization followed by ice removal, resulting in 3D co-continuous structures that exhibit rapid thermal responsiveness and inherent hydrophobic properties. Central to this innovation is an anisotropic device inspired by xylem vessel architecture, which functions as a nocturnal water channel valve, drawing water upwards during the night and releasing it at dawn. This system achieves remarkable efficiency, with water pumping rates ranging from 78% to 92%, and the volume of pumped water surpassing the mass of the material by a factor of 2 to 3 per cycle. Furthermore, the integration of water-purifying hydrogels enhances the system's functionality by effectively removing dye and oil contaminants. This unpowered system not only represents a cost-effective and environmentally compatible solution but also holds the potential to transform global water management practices.

Electrochemical oxidation of low concentration methane on Pt/Pt and Pt/CP under ambient conditions

Dr Ting Wu[1]
[1]Lincoln Agritech Ltd, Christchurch, New Zealand

Session 10B: Materials for Environmental and Water Management, Dobson 1, February 13, 2025, 10:40 - 12:45

Methane (CH4) is one of the main greenhouse gases as well as a clean and alternative energy source. Conversion and utilization of CH4 will contribute significantly to reducing global warming. However, CH4 utilization is challenging and energy intensive due to its stable chemical structure and low concentration in the atmosphere. Significant effort has been devoted, for instance, direct CH4 electrochemical partial conversion to methanol can be achieved using metal oxides as electrocatalysts under ambient conditions. Nevertheless, majority of the studies were conducted using pure methane as reactant and complicated metal oxides with/without cocatalysts were required. For industrial applications, simple catalyst fabrication and low concentration CH4 conversion and utilization are more practical.

Alternatively, a less explored and more straightforward approach is full oxidation to carbon dioxide (CO2) via “potential-dynamic” using platinum (Pt) as electrocatalyst. In this work, we activate and convert low concentration CH4 to CO2 under ambient conditions. Pt foil and carbon paper were coated with Pt particles (Pt/Pt and Pt/CP) via electrochemical deposition for CH4 oxidation. An oxidation potential was applied to electrochemically activate methane and followed by anodic cyclic voltammogram to fully oxidize activated CH4 to CO2. It was found that Pt/CP displayed approximately 10-time higher catalytic activity than Pt/Pt and this method can covert CH4 with different concentrations as low as 200 ppm. This study provides enhanced understanding of electrochemical methane oxidation with low concentration at low temperature. It offers a promising and cost-effective approach for methane oxidation catalysts optimization and future CH4 full utilization.

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Highly efficient zeolite supported Au-Pt alloy nanoparticles for long-term removal of ethylene at 0 degree C

Dr Mingyue Lin[1], Professor Toru Murayama[2], Professor Guangli Xiu[1]
[1]East China University of Science And Technology, Shanghai, China, [2]Hokkaido University, Sapporo, Japan

Session 10B: Materials for Environmental and Water Management, Dobson 1, February 13, 2025, 10:40 - 12:45

Ethylene is a natural gaseous plant hormone which will accelerate the food aging and quality deterioration even in the cold chain transportation and storage. Catalytic removal of ethylene is an ideal method, however, current reported catalysts suffered the deactivation within 2 hours at around 0 oC [1,2]. Solving the poor stability of catalyst is the key.

In this study, we report a gold-platinum (Au-Pt) alloy nanoparticles (NPs) catalyst (Au54Pt46/ZHM20) for highly efficient ethylene removal at 0 oC with a long-term stability [3]. Au54Pt46/ZHM20 showed robust C2H4 (of 50 ppm) removal capacity (initially more than 80%) at 0 oC for 15 days (360 h) and that the performance of the used catalysts would be fully recovered by heat treatment. This catalyst showed two stages of C2H4 removal: the first stage was attributed to the adsorption of C2H4 and the second could be due to the catalytic conversion of C2H4 to intermediates on Au54Pt46/ZHM20. Investigations by in-situ diffuse reflectance infrared Fourier transform (DRIFT) spectroscopy of C2H4 oxidation and online temperature programmed desorption measurements of the spent catalyst suggested that the Au-Pt nanoalloys favor the formation of acetic acid (AcOH) from selective ethylene oxidation. And this on-site-formed acetate intermediate would partially cover the catalyst surface at 0 oC, thus exposing active sites to prolong the continuous and effective C2H4 removal.

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Deep Eutectic Solvent (DES) as Green Absorbent for Scrubbing of Aromatic VOCs in Newly Decoration House: Formula Screening Using COSMO-RS

Ms. Yu-Hsuan Chang[1], Mr. Yu-Lin Cheng[1], Mr. Deng-Sen Chang[1], Mr. Yu-Chen Tseng[1], Mr. Yu-Ming Huang[2], A/Prof Min-hao Yuan[1]

[1]Department of Occupational Safety and Health, China Medical University, Taichung, Taiwan, [2]Department of Chemistry, National Taiwan University, Taipei, Taiwan

Session 10B: Materials for Environmental and Water Management, Dobson 1, February 13, 2025, 10:40 - 12:45

The indoor air in newly decorated houses often contains aromatic volatile organic compounds (VOCs), which, at high concentrations, may pose significant health risks. This study investigates common aromatic compounds present in indoor environments, including benzene, toluene, and naphthalene. The COSMO-RS (Conductor-like Screening Model for Real Solvents) theoretical calculation method was employed to evaluate Deep Eutectic Solvent (DES) formulations as green absorbents. A total of 23 hydrogen bond acceptors (HBAs) and 26 hydrogen bond donors (HBDs) were used, resulting in 598 DES combinations. The Henry constant (HC) and solvent capacity (SC) for each VOC were theoretically calculated.

At 25 °C, 101 kPa, and a 1:3 molar ratio of HBA to HBD, the HC and SC index results for toluene indicated that phenolic compounds and ammonium salts performed optimally among the HBAs, with thymol and tetrabutylammonium chloride (TBAC) demonstrating superior affinity for toluene's benzene ring structure. For HBDs, phenols, carboxylic acids, and alcohols were the top performers, especially phenyl hydroxide (PH) and 1-octanol (OctN), which showed enhanced affinity with the CH3 functional group in toluene.

The COSMO-RS simulation results for benzene, toluene, and naphthalene revealed that the best HBAs, based on the SC index, were tetrapropylammonium chloride (TPAC), TBAC, and tetrabutylammonium bromide (TBAB), while the top-performing HBDs were OctN, decanoic acid (DecA), and PH. These HBA-HBD combinations also demonstrated strong performance in terms of HC, making them ideal candidates for DES formulations designed to absorb aromatic VOCs commonly found in indoor environments.

Computational insight into the chemical processes underpinning a humidity driven molten carbonate membrane for direct air capture of carbon dioxide

Professor Patricia Hunt[1]
[1]Victoria University of Wellington, Wellington, New Zealand

Session 10C: Gas separation, concentration and CO2 ultisation, Dobson 2, February 13, 2025, 10:40 - 12:45

It is well established that CO_2 is the main contributor to climate change and that current efforts to reduce greenhouse gases will not be sufficient to keep a global temperature rise below 1.5ºC, or limit the climate impact of more extreme events such as wildfires, flooding or storms. Meeting climate goals will now also require CO_2 to be removed from the air. Some CO_2 can be captured at source (for example at a steel plant, power station or biorefining process). However, once CO_2 is in the atmosphere the problem is significantly more challenging. CO_2 is present in the air at a very dilute concentration, the absorption of CO_2 is generally an energetically uphill process and the system must work against a CO_2 concentration gradient. We have been exploring the potential for a molten carbonate membrane in combination with an ambient humidity difference to capture and concentrate CO_2 from the air. Engineering studies, under varying operational conditions, have proven the efficacy of our membrane reactor. However, there is very limited knowledge of how such a membrane works at the molecular level. At the engineering level simplified atom balance equations are almost universally presented, which cannot provide a clear understanding of the molecular species that might be involved. We have undertaken a molecular level DFT study exploring the potential chemical species that can form and have developed a mechanistic profile for H_2O facilitated uptake and transport of CO_2 within a (M= Li, Na, K eutectic) M_2CO_3 molten salt membrane operating at 550ºC.[1]

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Fundamental developments toward robust high-permeance ZIF-62 glass membranes

Dr Matthew Cowan[1], Dana M. Stone[1], Dr Sarah E. Morgan[2], Mai O. Abdelmigeed[2], Jimmy Nguyen[2], Professor Thomas D. Bennett[3], Professor Gregory Parsons[2]
[1]University Of Canterbury, Christchurch, New Zealand, [2]North Carolina State University, , USA, [3]Department of Materials Science and Metallurgy, University of Cambridge, Cambridge, United Kingdom

Session 10C: Gas separation, concentration and CO2 ultisation, Dobson 2, February 13, 2025, 10:40 - 12:45

This presentation reports investigation of two fundamental aspects towards preparing thin-film of MOF glasses.

The first aspect is controlling the thickness of the MOF membrane. We established that atomic layer deposition (ALD) of zinc oxide lends excellent control over the thickness and localization of resultant polycrystalline and glass zeolitic imidazole framework-62 (ZIF-62) thin-films within tubular α-alumina supports. Through the reduction of the chamber pressure and dose times during zinc oxide deposition, the resultant ZIF-62 films are reduced from 38 µm to 16 µm, while the presence of sporadic ZIF-62 (previously forming as far as 280 µm into the support) is prevented. Furthermore, the glass transformation shows a secondary reduction in film thickness from 16 to 2 µm.

The second aspect is a systematic examination of the relationship between melt time and temperature with the morphological changes, shown by microscope images of crystals agglomerating via melting, and porosity retention of ZIF-62 glasses shown through positron annihilation lifetime spectroscopy.

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Novel Hybrid Anion-Pillared MOFs For Strategic Gas Separations

Miss Sydnee Koia[1,2], Dr Nathan Harvey-Reid[1,2], Dr Soumya Mukherjee[3], Dr Paul Kruger[1,2]
[1]University of Canterbury, Christchurch, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand, [3]University of Limerick, Limerick, Ireland

Session 10C: Gas separation, concentration and CO2 ultisation, Dobson 2, February 13, 2025, 10:40 - 12:45

The ongoing development of modern society requires extensive quantities of energy, the majority of which comes from burning fossil fuels.1,2 This greatly contributes to the emission of greenhouse gases, such as CO2, which drive climate change.3 It is unlikely that environmentally-friendlier fuels will completely supersede the need for fossil fuels for the foreseeable future; therefore, reducing concentrated and atmospheric CO2 emissions from point sources and in the atmosphere is an urgent priority.

Further, regarding the large anthropogenic energy demand, industrial gas separations and purifications are critical, but energy-intensive, processes to generate many important fuels and polymers. This energy penalty arises due to the challenge of efficiently separating a target gas molecule from its highly similar impurities.4

Metal-organic frameworks (MOFs) are a promising class of porous coordination compounds to address these challenges in gas separations, however they can suffer a 'trade-off' between selectivity and uptake capacity.5 A subset of conventional MOFs, hybrid anion-pillared MOFs, have emerged amongst the top performing materials to address this compromise, owing to the impact of the anionic pillar through enhancement of framework tunability and introduction of strong electrostatic interactions.4

We report the synthesis, characterisation and gas adsorption performances of novel anion-pillared MOFs which have addressed the uptake-selectivity trade-off. This work highlights the impact of varying the anionic pillar on gas adsorption behaviour, underpinning the effect of subtle changes to the MOF building blocks in yielding significant improvements in their gas adsorption performances.

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Analogues of MUF-16 that further enhance CO2 capture performance in industrial applications

Ms Elnaz Jangodaz[1,2], Professor Shane G. Telfer[1,2]
[1]Massey University, Palmerston North, New Zealand, [2]Captivate Technology Ltd, Palmerston North, New Zealand

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MUF-16 (MUF = Massey University Framework) is an excellent adsorbent for CO_2 capture that is being commercialized by Captivate Technology to address point-source emissions.[1] MUF-16 is a porous metal-organic framework (MOF) known for its high CO_2 selectivity over nitrogen and methane, tolerance to impurities, and long-term stability. It can be produced on a large scale from inexpensive precursors, being prepared simply by combining 5-aminoisophthalic acid (H_2aip) and cobalt (II) acetate.

Our recent advances on MUF-16 include measuring its SO_2 uptake and investigating its flexibility upon hydrocarbon adsorption.[2]-[4] In addition, we investigated whether the carbon capture performance of MUF-16 could be enhanced by introducing new ligands into its structure.[2] Such mixed-linker MOFs are often referred to as 'multivariate' MOFs. The 'anchoring' ligand is H_2aip, as used in MUF-16 itself, and the second ligand engineers the pores of MUF-16 in terms of their shape, size and physicochemical characteristics. Our results indicate that these MUF-16 analogues can:

- Significantly enhance CO_2 capture capacity at low partial pressures, suitable for point-source applications with CO_2 concentrations as low as 1% and becoming realistic for direct air capture (DAC).
- Effectively suppress the capacity of other gases such as N_2 and CH_4 to enhance selectivity.
- Increase water vapor tolerance, reducing the H_2O capacity by approximately 30% at low relative humidities.

These developments address critical industrial needs by enabling efficient CO_2 capture from low concentration sources and mitigating challenges associated with humid flue gases. By improving the selectivity and capacity of MUF-16 while reducing its affinity for other gases, we provide a robust solution for industrial applications where both high efficiency and resilience to operating conditions are essential.

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Development of Defect-Free Metal-Organic Framework (MOF) Membranes for Enhanced Gas Separation performance

Mr Harikrishnan Raghavan[1,2], Dr. Matthew Cowan[1,2]
[1]University Of Canterbury, Christchurch, New Zealand, [2]MacDiarmid Institute, NewZealand

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Development of Defect-Free Metal-Organic Framework (MOF) Membranes for Enhanced Gas Separation performance

This work brings the large-scale application of MOF membranes in the industrial gas separation process closer by providing a generalizable method for fabricating defect-free MOF membranes.
Owing to their well-defined pore structures and flexibility, Metal-organic frameworks (MOFs) have gained significant interest in the field of gas separation. However, fabricating mechanically stable defect-free MOF membrane layers is still a challenge. 1 Because of their crystalline nature, MOFs form grain boundaries at crystal-crystal interfaces. 2 These grain-boundary defects provide high-permeance non-selective transport pathways for small molecules, severely limiting membrane performance. 3 Hence, growing thin, defect-free layers of MOF over sufficient areas is extremely difficult.

This study introduces a novel, generalisable method for fabricating mechanically robust, high-performance, defect-free MOF membranes confined within the pores of tubular ceramic supports suitable for application in gas separation processes. These membranes, and the fabrication technique, have potential applications in the purification of hydrogen and carbon dioxide, which can significantly improve energy efficiency and reduce carbon footprint.

Detailed characterisation of the as-fabricated membranes using scanning electron microscopy (SEM) shows that the intercrystalline boundary defects are successfully filled under specific conditions. Subsequent gas testing results confirm a marked improvement in separation performances post-treatment.

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Development of thermoelectric materials & devices for energy saving and IoT energy harvesting

Professor Takao Mori[1,2]
[1]National Institute for Materials Science (NIMS), Tsukuba, Japan, [2]University of Tsukuba, Tsukuba, Japan

Session 10D: Thermo- and piezo- electric materials, Dobson 3, February 13, 2025, 10:40 - 12:45

Development of thermoelectric materials is important, for energy saving via waste heat power generation, and to power innumerable IoT sensors. To achieve enhanced thermoelectrics, it is necessary to overcome conventional tradeoffs between key properties, namely, between thermal and electrical conductivity, and between Seebeck coefficient and electrical conductivity [1]. I will present several mechanisms, involving band engineering, phonon engineering, defect engineering, etc., where we have been able to achieve this.

For example, utilizing of Anderson localized states has recently led to notable enhancement of the Seebeck coefficients in ZnO and Fe_2VAl Heuslers, for example [2]. In addition to traditional nano-microstructuring, partially occupied atomic sites, or heterogeneous bonding in mixed anion compounds have been respectively shown to result in exceptional low lattice thermal conductivity [3]. A striking interstitial and grain boundary control led to $Mg_3(Sb,Bi)_2$-type being enhanced to rival long time thermoelectric champion bismuth telluride for both power generation [4] and cooling [5]. Recently, a single element device of doped Mg_3Sb_2 has achieved efficiency above 12% [6].

I will also describe recent advancements we have made in various formats of thermoelectric power generation modules, such as bulk, thin film, flexible, and applications.

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Strain induced Flexible Piezoelectric device employing Semiconducting Nanowire Network

Dr Shruti Sharma[1], Dr Muriel Braccini[2], Dr Fabien Volpi[2], Dr Gustavo Ardila[3], Dr Céline Ternon[1]
[1]Univ. Grenoble Alpes, CNRS, Grenoble INP, LMGP, Grenoble, France, [2]Univ. Grenoble Alpes, CNRS, Grenoble INP, SIMaP, Grenoble, France, [3]Univ. Grenoble Alpes, CNRS, Grenoble INP, Croma, Grenoble, France

Session 10D: Thermo- and piezo- electric materials, Dobson 3, February 13, 2025, 10:40 - 12:45

The development of functional devices compatible with standard microelectronic processes is central to the More-than-Moore and Beyond-CMOS electronic fields. Devices based on nanowires (NWs) are very promising, but their integration remains complex and submitted to variability limiting the potential scalability. Flexible electronics is a field in which the standard microelectronic industry struggles to propose a solution. Despite tremendous progress, organic materials remain highly sensitive to oxygen and humidity and deteriorate under UV irradiation, thus limiting their long-term operation. Recently, we have demonstrated that semiconducting nanonets, two-dimensional networks of randomly oriented nanowires, provide an easy-to-process single answer to develop flexible electronics and NW based devices [1]. However, when dealing with piezoelectric NWs such as ZnO-NWs, there is limited knowledge available regarding the piezotronic behaviour of these nanonets, that is to say, the electronic transport phenomena that occur in this piezoelectric material.

Here we show that, despite the random orientation of the nanowires, the devices based on ZnO nanonets integrated on flexible substrates exhibit piezoproperties. Upon successful integration of nanonets to form resistor devices, their electro-mechanical behaviour was studied under application of strain of varied magnitude and orientation, elongation and compression, using a traction- and bending- based setup. The results obtained suggest that the material is very well suited to contributing to piezotronics [2]. As a result, we were able to build a piezoelectric transistor based on ZnO nanonet which turn on and off with strain. With Ion/Ioff ratio as high as 10^5, the performance is highly promising.

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Mitigating Triboelectric Effects in Piezoelectric Signal Measurements

Mr Alireza Akbarinejad[1], Dr Holger Fiedler[2], Ms Jade Nguyen[1], Mr Zifan Li[1], Mr Donn Adam Gito[1], Dr Peter Sherrell[4], Dr Amanda Ellis[3], Dr Kean Aw[1], Dr Jenny Malmstrom[1]
[1]The University of Auckland, Auckland, New Zealand, [2]GNS Science, National Isotope Centre, Wellington, New Zealand, [3]The University of Melbourne, Melbourne, Australia, [4]RMIT University, Melbourne, Australia

Session 10D: Thermo- and piezo- electric materials, Dobson 3, February 13, 2025, 10:40 - 12:45

The significance of piezoelectric materials lies in their unique ability to convert mechanical energy into electrical signals.1 However, accurately measuring the piezoelectric electric signal is often complicated by triboelectric interference, which arises from unwanted electrical charges generated by friction between materials.2 In this study, we thoroughly investigate the signal output from different materials, including those with strong, moderate, and no piezoelectric properties.3 The testing process involves tapping and compressing (33 direction) as well as stretching (31 direction) the materials, both in encapsulated and non-encapsulated forms. Our findings reveal significant voltage outputs across all materials during tapping, emphasizing the dominance of triboelectric signals in this mode. Most of this triboelectric signal is eliminated during compression-based mechanical stressing, while in stretching mode, triboelectric interference is minimal. Additionally, our results indicate that encapsulating the materials with soft elastomers significantly increases triboelectric signals during tapping. These findings have important implications for improving the design and performance of piezoelectric-triboelectric devices in practical applications.

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Defects induced high thermoelectric power factor in sustainable thermoelectric materials

Dr Peter Murmu[1], Dr John Kennedy[1,2], Mr Martin Markwitz[1,2], Prof Takao Mori[3,4]
[1]National Isotope Centre, GNS Science, Lower Hutt, New Zealand, [2]The MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand, [3]International Center for Materials Nanoarchitectonics (WPI-MANA), National Institute for Materials Science (NIMS), Tsukuba, Japan, [4]Graduate School of Pure and Applied Science, University of Tsukuba, Tsukuba, Japan

Session 10D: Thermo- and piezo- electric materials, Dobson 3, February 13, 2025, 10:40 - 12:45

Thermoelectric materials enable clean energy harvesting by converting heat into electricity via the Seebeck effect for low-energy technology[1]. There is a growing demand for the development of sustainable thermoelectric materials for low-to-intermediate temperature applications. Copper and zinc-based semiconductors are non-toxic, abundant, and low-cost, making them promising candidates for sustainable thermoelectric materials. However, their practical application is hindered by low electrical conductivity (σ), poor stability, and gradual decomposition, which reduce energy conversion efficiency and result in a low power factor ($\alpha^2\sigma$), where α is the Seebeck coefficient.

In this paper, we elucidate the role of defect and dopant complexes in achieving high thermoelectric power factors in copper iodide (CuI)[2,3], indium-tin-oxide (ITO)[4], and zinc antimonide (Zn_4Sb_3)[5] thin films. Microstructural characterization revealed polycrystalline γ-CuI, bixbyite-In_2O_3, and β-Zn_4Sb_3 phases. Annealing-induced defects and secondary phases were found to be beneficial for the electrical properties of these films. Chalcogen element doping was performed to enhance the thermoelectric power factor of CuI films[2]. Implantation of 30 keV $^{79}Se^+$ into CuI films resulted in a simultaneous increase in α and σ, leading to an ~86% increase in the thermoelectric power factor. Density functional theory and Monte-Carlo calculations revealed that the substitutional Se at the I site (SeI) and copper vacancy (VCu) defect complex exhibited a shallower acceptor transition than isolated SeI and VCu defects. Our results demonstrate that annealing and implantation generate point defects favorable for forming defect complexes with the dopant, simultaneously increasing α and σ, and resulting in a high power factor.

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Increasing the thermoelectric power of CuI by defect engineering with ion implantation

Mr Martin Markwitz[1,2,3], Dr Peter Murmu[2], Professor Takao Mori[4,5], Adjunct Professor John Kennedy[2,3], Associate Professor Ben Ruck[1,3]
[1]School of Chemical and Physical Sciences, Victoria University of Wellington, Wellington, New Zealand, [2]National Isotope Centre, GNS Science, Wellington, New Zealand, [3]The MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, Wellington, New Zealand, [4]International Center for Materials Nanoarchitectonics (WPI-MANA), National Institute for Materials Science (NIMS), Tsukuba, Japan, [5]Graduate School of Pure and Applied Science, University of Tsukuba, Tsukuba, Japan

Session 10D: Thermo- and piezo- electric materials, Dobson 3, February 13, 2025, 10:40 - 12:45

Copper(I) iodide, CuI, is the leading p-type non-toxic earth-abundant semiconducting material for transparent electronics [1]. CuI is actively garnering significant attention for its highly tunable optoelectronic and thermoelectric properties through control of its carrier concentration [2]. In this study we increase the electrical conductivity of CuI thin films by implantation with chemically inert noble gas ions (Ne, Ar, and Xe) from the production of beneficial point defects. We find a 53 % increase in electrical conductivity from 76±2 S/cm to 116±3 S/cm without detrimentally affecting the Seebeck coefficient or carrier mobility. This conductivity variation led to an 80 % improvement of the thermoelectric power factor to 578±58 $\mu W/mK^2$ from the as-deposited average of 322±32 $\mu W/mK^2$. The cause of the increased power factor is a 77 % enhanced carrier concentration, increasing from the already high $6.5\times10^{19}\pm0.1\times10^{19}$ /cm³ to an average of $11.5\times10^{19}\pm0.4\times10^{19}$ /cm³. This research builds on previously implanted chalcogenide dopants in CuI, which resulted in a mixture of beneficial and detrimental effects [3,4,5]. Density functional theory calculations were conducted to investigate Frenkel pairs and their binding energies in CuI, which were produced by ion implantation. This work provides an important step forward in the development of CuI as a commercially viable transparent conducting material with beneficial point defects and defect complexes.

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Soft Magnetic Materials for Inductive Power Transfer to Electric Vehicles

Professor Nick Long[1], Dr Neena Devi[1], Dr Shen Chong[1], Bill Trompetter[2], John V. Kennedy[2], Alexander Bailey[3], Wenting Zhang[3], Dr Seho Kim[3]
[1]Paihau-Robinson Research Institute, Victoria University of Wellington, Lower Hutt, New Zealand, [2]GNS Science, Lower Hutt, New Zealand, [3]Department of Electrical, Computer and Software Engineering, University of Auckland, Auckland, New Zealand

Session 10D: Thermo- and piezo- electric materials, Dobson 3, February 13, 2025, 10:40 - 12:45

Inductive power transfer to electric vehicles simplifies recharging. Rather than through a power cable, a vehicle draws power from a charging pad when positioned over the pad. The process could be stationary in a home garage or commercial parking space, or while in motion in a motorway charging lane [1]. The efficiency of inductive charging is important not only for cost effectiveness and speed of charging but also for thermal management of the transmit and receive pads. A key component of achieving efficiency is the use of high permeability soft magnetic materials to concentrate magnetic flux in the gap between transmit and receive coils [2,3]. We report results on permeability and magnetic losses of soft magnetic composites incorporating crushed ferrites and iron sand. A simple theoretical analysis shows that for isotropic composites, the relative permeability is limited to the order of 100. The results show that our best materials approach this value at high concentrations. Greater flux concentration can be achieved by incorporating anisotropic sheets of nanocrystalline magnetic alloys. The downside of these materials is the metallic conductivity leading to eddy current losses. We have experimented with deliberately fracturing the alloys to increase resistance and reduce eddy current losses. We also report the results of chemical treatments to reduce conductivity through oxidising grain boundaries. We report the conductivities for different fracturing and chemical treatments. We present permeability and loss measurements on fractured nanocrystalline sheets to inform the trade-off between improved magnetic coupling and electrical losses within the magnetic materials.

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Exploring Non-Classical Properties of Amyloid Fibrils

Mr Donn Adam Gito[1,2], Dr Alireza Akbarinejad[1,2], Dr Alex Dixon[3], Dr Thomas Loho[1], Dr Michel Nieuwoudt[1,2,4], Mrs Qun Chen[1], Dr Alexander Elliot[2,3], Dr Laura Domigan[1,2], Dr Jenny Malmström[1,2]
[1]Department of Chemical and Materials Engineering, Faculty of Engineering, The University of Auckland, Auckland, New Zealand, [2]The MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand, [3]The Auckland Bioengineering Institute, The University of Auckland, Auckland, New Zealand, [4]School of Chemical Sciences, The University of Auckland, Auckland, New Zealand

Session 10D: Thermo- and piezo- electric materials, Dobson 3, February 13, 2025, 10:40 - 12:45

The fibrous proteins collagen, silk fibroin, and keratin share a unique functional similarity that is more commonly found in inorganic crystalline materials. [1], [2] These proteins produce electrical charges in response to applied stress, demonstrating piezoelectricity. However, in recent discoveries, non-fibrous crystallised proteins showed a similar behaviour. [3], [4] Hence, creating ambiguity regarding the type of protein structure and how much influence it has on a protein's piezoelectric behaviour. Lysozyme is an example of a protein shown to be piezoelectric when crystallised. In our research, we are looking into how the piezoelectric property of the globular protein lysozyme changes when converted into fibrils with a different secondary structure. Our results show that even in its amyloid fibril form, when assembled into freestanding films, lysozyme exhibits a low but measurable longitudinal piezoelectric response of 1.4 ± 0.1 pC of charge for every Newton force. Within these films, we also discovered complex interactions between the fibrils and added plasticising agents, as well as the film's light polarising abilities due to the fibril's circumferential alignment. Overall, these initial results demonstrate the potential of using amyloid fibrils, which can be formed from various proteins, as a source for creating a bulk self-assembled piezoelectric material. Now, we are investigating the use of these piezoelectric fibrils and films as energy-harvesting devices. Our current work also looks into optimising the protein films' piezoelectric output through the incorporation of complex inorganic materials such as polyoxometalates.

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Ultrafast Coulomb Interactions in Organic Semiconductors for Next Generation Solar Panels

Dr Michael Price[1]
[1]University Of Bristol, Bristol, United Kingdom

Session 10E: Photovoltaic, light harvesting and optical materials, Dobson 4, February 13, 2025, 10:40 - 12:45

Next generation photovoltaics promise cheap and versatile solar energy – particularly for new applications such as semi-transparent solar windows. Materials chemists have made great progress in designing new and easily processable semiconductors over the last two decades. Device physics and ultrafast spectroscopy have guided this progress, particularly in the fields of metal halide perovskites, and molecular organic semiconductors. I will speak about previous work which generated new understanding of fundamental photophysical processes in these materials, and our efforts at implementing this understanding in useful optoelectronic devices (solar cells, LEDs and lasers).

I will outline recent developments in the field of 'fused ring electron acceptors' (FREAs) for organic photovoltaics[1][2], and focus on the crucial interplay of charge photogeneration versus recombination in dictating device efficiency. The Coulombic forces governing the behaviour and lifetimes of electrons, holes and excitons in these materials still generate active debate, and are difficult to measure, and hence are usefully studied via ultrafast laser spectroscopies. Based on some of our spectroscopic findings, I will suggest new approaches to enhancing organic photovoltaic efficiency, such as through molecular doping and crystal structure engineering.

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Non-Volatile Solid Additives for High-Efficient Eco-Friendly Organic Photovoltaic Cells

Dr Do Hui Kim[1], Professor Shinuk Cho[1]
[1]University Of Ulsan, Ulsan, South Korea

Session 10E: Photovoltaic, light harvesting and optical materials, Dobson 4, February 13, 2025, 10:40 - 12:45

As organic photovoltaics (OPVs) have become more commercially viable in recent years, with power conversion efficiencies (PCEs) exceeding 20%, the importance of environmental sustainability has grown significantly. Most eco-friendly OPVs have primarily focused on replacing solvents in the photoactive layer with environmentally benign alternatives, yet they still rely on harmful additives to modulate the morphology of the photoactive layer. This reliance remains a major obstacle to achieving fully environmentally friendly OPVs. In this study, we propose a fully eco-friendly OPV that employs environmentally harmless materials not only for solvents but also for additives used in the formation of the phase-separated morphology of the photoactive layer. To elucidate the effect of volatility on the morphology of the photoactive layer, we systematically investigated its morphological characteristics using eco-friendly solid additives with varying boiling points. As a result, the non-volatile eco-friendly solid additive, 4,4'-dihydroxybiphenyl (DBP), facilitated the formation of an optimal photoactive layer morphology, characterized by enhanced crystallinity due to high miscibility between the donor and acceptor materials. This led to the development of a fully eco-friendly OPV with a high PCE of 17.78%.

Resolving the emissive intermediate in singlet fission with magnetic fields

Mr Damon De Clercq[1], Dr Jiale Feng[1], Dr Parisa Hosseinabadi[2], Dr Ben Carwithen[1], Dr Michael Nielsen[2], Dr Matthew Brett[1], Dr Shyamal Prasad[1], Dr Adam Farahani[3], Dr Samuel Sanders[4], Prof. jonathon Beves[1], Prof. N.J. Ekins-Daukes[2], Prof. Jared Cole[5], Prof. Pall Thordarson[3], Associate Prof. David Huang[6], Associate Prof. Murad Tayebjee[2], Prof Timothy Schmidt[1]
[1]ARC Centre of Excellence in Exciton Science, School of Chemistry, UNSW Sydney, Sydney, Australia, [2]School of Photovoltaic and Renewable Energy Engineering, UNSW Sydney, Sydney, Australia, [3]The UNSW RNA Institute, The Australian Centre for Nanomedicine, School of Chemistry, UNSW Sydney , Sydney, Australia, [4]Rowland Institute at Harvard University, Cambridge, USA, [5]ARC Centre of Excellence in Exciton Science, School of Science, RMIT University, Melbourne, Australia, [6]Department of Chemistry, School of Physics, Chemistry and Earth Sciences, The University of Adelaide, Adelaide, Australia

Session 10E: Photovoltaic, light harvesting and optical materials, Dobson 4, February 13, 2025, 10:40 - 12:45

Singlet fission offers a way to overcome the detailed balance limit in silicon photovoltaics by addressing thermalization losses. This process, which occurs in adjacent chromophores, describes the partitioning of the singlet excited state into two low-energy triplet excitons via a triplet pair intermediate ^{1}(TT). If the triplet state energy is greater than the 1.1 eV bandgap of silicon, the triplet excitons in the organic semiconductor can transfer to silicon. Such a device could realize efficiencies of 45%.

Tetracene was recently shown to undergo triplet transfer to silicon. This demonstration was a major step towards the realization of a working singlet fission device.[1] However, tetracene is not an ideal chromophore as the singlet fission yield is not unity (120% out of 200%) and the triplet energy (1.1 eV) is on the silicon band edge. The field therefore requires new chromophores that have yields closer to unity and greater triplet energies.

To design new chromophores a clear understanding of the role of the excimer state, and the nature of the triplet-pair state in in singlet fission is required. This presentation will discuss our recent results in resolving the emissive intermediate state in singlet fission.[2] I will present transient photoluminescence and spectrally resolved magneto-photoluminescence data which identifies an emissive species that is distinct from the excimer state. Our results confirm that the excimer is a trap state and unites the view that the ^{1}(TT) state is an emissive intermediate in singlet fission.

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Morphological control of Y6 thin films reveals charge transfer generation is facilitated by co-facial interactions.

Ms Aditi Kumar[1,2], Dr. Rohan Hudson[3], Dr. Bo-Han Chen[6], Mr. Nikita Shumilov[1,2], Mr. Chao-Yang Lin[2,4,5], Prof. Trevor Smith[3], Dr. Nathaniel Davis[1,2,5], Prof. Eric Le Ru[1,2], Prof. Yu-Chiang Chao[8], Prof. Shang-Da Yang[6,7], Dr. Michael Price[9], Dr. Kai Chen[2,4,5], Dr. Paul Hume[1,2], Prof. Justin Hodgkiss[1,2]
[1]School of Chemical and Physical Sciences, Victoria University of Wellington, Wellington , New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand, [3]ARC Centre of Excellence in Exciton Science, School of Chemistry, University of Melbourne, Victoria, Australia, [4]Robinson Research Institute, Faculty of Engineering, Victoria University of Wellington, Wellington, New Zealand, [5]The Dodd-Walls Centre for Photonic and Quantum Technologies, University of Otago, Dunedin, New Zealand, [6]Institute of Photonics Technologies, National Tsing Hua University, Hsinchu, Taiwan, [7]College of Semiconductor Research, National Tsing Hua University, Hsinshu, Taiwan, [8]Department of Physics, National Taiwan Normal University, Taipei, Taiwan, [9]School of Chemistry, University of Bristol, Bristol, United Kingdom

Session 10E: Photovoltaic, light harvesting and optical materials, Dobson 4, February 13, 2025, 10:40 - 12:45

The organic semiconductor Y6 has been used extensively as an acceptor in organic photovoltaic devices, yielding high efficiencies. Its unique properties include a high refractive index, intrinsic exciton dissociation because of its low exciton binding energy and intermolecular arrangement, and barrierless charge generation in bulk heterojunctions. However, the direct impact of crystal packing morphology on the photophysics of Y6-based materials has remained elusive, hindering further development of both heterojunction and homojunction devices. Herein, we study and characterize the photogenerated species in multiple distinct Y6 crystal packing geometries via transient absorption spectroscopy. We show that 'co-facial' dimers in the bulk are responsible for the observed generation of charge-transfer (CT) states /charge pairs in neat films of Y6, but the presence of these dimers doesn't influence the charge-transfer state lifetime. We find that exciton dissociation can be switched on/off by controlling co-facial interactions. We further show that by performing additive induced optimisation of co-facial interactions, we can tune the nature of CT generation to be primarily intrinsic as opposed to resulting from bimolecular events. Our findings provide fundamental knowledge on structure-property relationships with relevance to device optimization. As efficiencies achieved by the random mixing technique of the bulk heterojunction plateau, our work highlights an alternative approach and the advantage of systematically studying packing within neat domains to gain better control over molecular photophysics.

Optimizing growth of self-assembled aluminide stacks for optical applications

Mr Angelo Vitaliti[1], AProf Matthew Arnold[1]
[1]University Of Technology Sydney, Sydney, Australia

Session 10E: Photovoltaic, light harvesting and optical materials, Dobson 4, February 13, 2025, 10:40 - 12:45

Self-assembled nanostructured thin films offer a facile route to accessing maximum design flexibility for optical filters, with advanced properties including polarization and directional selectivity. Recently, we demonstrated a new growth mode that exploits the low diffusion of co-sputtered aluminides for enhanced nanostructural stability, enabling high-yield fabrication of highly anisotropic layers at modest deposition angles[1]. When converted into the phase change material vanadium dioxide, these stacks enable advanced functionality such as thermally-configurable polarization and spectral filtering[2]. However, the as-deposited stacks include an unstructured layer that complicates optical design. Here we investigate the effect of larger deposition angle for improved design flexibility, demonstrating the feasibility of increased as-deposited transmission.

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Stretching Long-Lived Excited States Using Molecular Design, A Transient Resonance Raman Study.

Mr Samuel Harris[1], Dr Georgina Shillito[2], Dr Stephan Kupfer[2], Professor James Crowley[1], Professor Keith Gordon[1]
[1]University Of Otago, Dunedin, New Zealand, [2]Friedrich Schiller University, Jena, Germany

Session 10E: Photovoltaic, light harvesting and optical materials, Dobson 4, February 13, 2025, 10:40 - 12:45

Long-lived excited state behaviour is an important attribute for many photophysical applications, such as photocatalysis or photodynamic therapy. As such we have designed, synthesised and characterised a series of complex symmetrical Rhenium-based multidonor-acceptor dyes. The series contains two D-A-D style ligands, and 4 auxiliary tuning ligands, each complex exhibited a multitude of both metal-ligand charge transfer and intra-ligand charge transfer transitions. Across the series there was switching between the lowest energy excited states, as well as energy tuning, and the elongation of excited state lifetimes according to molecular architecture. To investigate these dyes, we used a conglomerate of spectroscopic techniques such as transient absorption, emission and resonance Raman spectroscopies. Additionally, we are utilising computational techniques to understand and support the spectroscopic results we observe.

Fundamental Properties and Device Applications of Square SnO2 Nanotubes

Mr Ryan Adams[1,3], Professor Martin Allen[1,3], Professor Roger Reeves[2,3]
[1]Department of Electrical and Computer Engineering, University of Canterbury, Christchurch, New Zealand,
[2]School of Physical and Chemical Sciences, University of Canterbury, Christchurch, New Zealand,
[3]MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand

Session 10E: Photovoltaic, light harvesting and optical materials, Dobson 4, February 13, 2025, 10:40 - 12:45

Tin dioxide (SnO_2) is a technologically-important transparent semiconducting oxide. Its wide (3.5 eV) bandgap combined with strong n-type electrical conductivity makes SnO_2 well-suited for ultraviolet optoelectronic devices and transparent electronics, while other properties such as a high surface electron density and donor-like oxygen vacancies enable a variety of gas sensing and electrocatalytic applications. We have developed a highly-scalable method of growing perfectly-square SnO_2 nanotubes using mist chemical vapour deposition[1]. These square nanotubes have a unique 90° geometry and exhibit high single crystallinity alongside large surface-to-volume ratios.

Synchrotron x-ray photoelectron spectroscopy has revealed the presence of an unusually strong 2-dimensional electron gas (2DEG) at the nanotube surface, produced by surface hydroxyl terminations. Unlike other oxide semiconductors, this 2DEG is sustained at high temperatures by the formation of donor-like in-plane oxygen vacancies[1]. While this is very useful in gas sensing and catalytic applications, a neutral surface electron density is better for optoelectronic devices and transparent electronics. We show that the surface electron density can be bi-directionally controlled for different applications through phosphonic acid and sulfur surface treatments.

We also report on electronic devices based on these square nanostructures. Single square SnO_2 nanotube Schottky diodes and field-effect transistors (FETs) were fabricated with large on/off current ratios of up to 10^7 and very low leakage currents, representing an important step towards utilising these structures in optoelectronic and gas sensing applications. We have also fabricated a range of electrolytically-gated square SnO_2 nanotube FETs which demonstrate strong paired-pulse facilitation, intended for neuromorphic and bio-sensing applications[2].

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CO2 Electro-Reduction: From Metallic Foams to Gas Diffusion Electrodes

Christina Roth[1], MIna Attia[1], Carl-Eric Hartwig[1], Philipp Hawe[1], Hendrik Hoffmann[1], Ralf Moos[1]
[1]University Of Bayreuth, Bayreuth, Germany

Keynote Session 17, Auditorium, February 13, 2025, 13:45 - 14:20

A future sustainable energy scenario relies on fossil-free electricity production and significant reduction of our greenhouse gas emissions. Indeed, carbon dioxide electroreduction (CO2RR) to either commodity chemicals or fuels may become an important puzzle piece in this setting. However, CO2 is a sluggish molecule and its reaction towards CO, formic acid or C2 products, such as ethene, is plagued by very similar overpotentials and a low selectivity. Most importantly, the careful selection of the electrocatalyst material, its oxidation degree, and surface morphology strongly defines the final product spectrum. While in the conversion of carbon dioxide to carbon monoxide Ag achieves faradaic efficiencies close to 100 %, for any reaction towards C2 products Cu is the material of choice. A fast, simple and scalable strategy to process highly active porous metal electrodes with increased surface area is the dynamic hydrogen bubble templation (DHBT) taking advantage of the (normally undesired) hydrogen evolution reaction (HER) in aqueous electrolyte. HER occurs simultaneously to metal deposition, so that the deposits grow around the evolving bubbles forming macro-porous layers and nanoscale interconnecting foam walls. Herein, we will demonstrate how the DHBT method can be used to produce model Ag and Cu electrodes with controlled morphology and porosity to be tested in H cells for the CO2RR within minutes. This strategy will then be transferred to gas diffusion electrodes, which allow for investigation in technically-relevant high current densities in dedicated flow cells.

Unveiling dynamic biotic-abiotic interactions in photosynthetic biohybrids

Weidong Zhang[1], Glenn Quek[1], Bin Liu[1], Guillermo Bazan[1], Xianwen Mao[1]
[1]National University of Singapore, Singapore

Keynote Session 18, Dobson 1, February 13, 2025, 13:45 - 14:20

Microbe–semiconductor biohybrids have recently emerged as a promising system for solar-to-chemical conversion due to the combination of high-selectivity chemical production by microbes and the efficient light-harvesting capabilities of inorganic semiconductors. Optimal performance of these biohybrids requires a mechanistic, quantitative understanding of dynamic biotic/abiotic interactions at the biotic/abiotic interface. However, these aspects are challenging to study through ensemble-averaged bulk measurements due to the ubiquitous heterogeneities of both constituents.1 In this work, we developed a multimodal functional imaging platform that combines super-resolution imaging and photocurrent mapping to probe biotic/abiotic interactions at single-cell and subcellular levels for an emerging type of photosynthetic biohybrids that consist of nitrogen-fixation bacteria and membrane-intercalating conjugated oligoelectrolytes. We uncover that the spatial distribution of conjugated oligoelectrolyte semiconductors in single bacterial cells can dynamically affect the aggregation state of biohybrids and their overall electron uptake capability. Our imaging tools and associated analytical frameworks provide a design principle to optimize the spatiotemporal distribution of photocatalytic materials in a nitrogen-fixation bacteria, enabling efficient and stable solar-to-chemical conversion.

Effect of cathodic potential in electrochemical CO2 reduction

Dr Lei Wang[1]
[1]National University of Singapore, Singapore, Singapore

Session 11A: CO2 reduction, Auditorium, February 13, 2025, 14:25 - 16:00

The electrochemical reduction of CO2 holds immense promise as a sustainable approach to mitigate greenhouse gas emissions and produce valuable chemical feedstocks. Therefore, great efforts have been dedicated to advancing this process, including the design of new catalysts through modifications in composition, facet, and morphology, as well as optimizing reaction microenvironments and reactor configurations. Despite that significant progress has been made, the unsatisfactory performance of electroreduction of CO2 under practical relevant conditions has hindered the practical implementation of this technology. In this presentation, we report the critical role of cathodic potential in modulating the selectivity, activity and even stability of CO2 reduction. Specifically, we will introduce a few of our recent discoveries: (1) potential-dependent activity, selectivity and stability of Cu-based CO2 reduction systems[1]; and (2) potential-dependent structural evolution of Pd-based catalyst during CO2 reduction to formate[2]; (3) potential-driven structural distortion of Co-Phthalocyanine in methanol production from CO2 electro-reduction[3]. Overall, through a combination of experimental investigations and theoretical modelling, we elucidate the intricate interplay between reaction kinetics, thermodynamics, and electrode surface properties. This study underscores the importance of considering cathodic potential as a crucial parameter in the design and optimization of electrochemical CO2 reduction systems, with significant implications for renewable energy conversion and carbon utilization technologies.

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The role of structural dynamics in liquid metal catalysts

Dr Charlie Ruffman[1]
[1]University Of Auckland, Auckland, New Zealand

Session 11A: CO2 reduction, Auditorium, February 13, 2025, 14:25 - 16:00

Gallium-based alloys are receiving growing attention as catalysts, as they showcase reactivity, selectivity, and long-term stability that often outclasses their solid heterogeneous counterparts.[1-3] These alloys – known as liquid metals – exist as liquids close to room temperature, thus combining the activity of traditional transition metal catalysts with the flexibility and self-healing nature of a liquid. In particular, Ga-In and Ga-Sn have previously showcased incredible (>95%) selectivity towards the electrochemical reduction of CO2 to formate, occurring only when the alloys are melted, not solid.[4]

In this presentation, density functional theory molecular dynamics simulations reveal the underlying mechanism for selectivity formate production, and explain why this occurs only on the liquid catalyst.[5,6,7] We find that CO_2 does not directly adsorb to the Ga-alloy surface, but instead is reduced indirectly by reaction with adsorbed hydrogen. This process can occurs favourably only when both CO_2 and H neighbour an In or Sn dopant site. Critically, adsorbed hydrogen is mobile only on the liquid metal, not the solid. Hydrogen's mobility due to the motion of the liquid atoms beneath, driving the adsorbate to reacting sites.[6,7] Therefore, the dynamic motion of liquid metal catalysts can underpin their unique reactivity. These results have far-reaching implications for any protonation reaction conducted with a liquid metal catalyst, suggesting they may offer a key to improved reactivity.

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Liquid metal chemistry towards CO2 reduction and other catalytic reactions

Professor Torben Daeneke[1]
[1]Rmit University, Melbourne, Australia

Session 11A: CO2 reduction, Auditorium, February 13, 2025, 14:25 - 16:00

Liquid metals are an emerging class of compounds that are liquid close to room temperature yet exhibit metallic conductivity. Liquid metals have found application in the design of flexible and reconfigurable electronics and more recently emerged as a platform for the synthesis of nano-structures as well as a unique class of catalysts that is extraordinarily resilient towards deactivation. In comparison to other liquids such as covalent solvents and ionic liquids, comparatively little is known about the chemistry that occurs inside molten metals. This talk covers the emerging picture of liquid metal chemistry and will report our most recent results on the fundamental processes that govern the behaviour of liquid metals. Following this, our work in the area of CO2 electroreduction, chemical looping of liquid metals to turn CO2 into graphene and the synthesis of NH3 will be covered.

Metal-Organic Frameworks for CO2 Electrocatalysis

Mr Shae Patel[1,2], Dr Luke Liu[1,2], Dr Kim McKelvey[1,2]
[1]Victoria University of Wellington, Wellington, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand

Session 11A: CO2 reduction, Auditorium, February 13, 2025, 14:25 - 16:00

Research into carbon dioxide (CO_2) reduction methods is crucial in reducing atmospheric CO_2 levels. Electrochemical CO_2 reduction is a promising method due to the implementation of renewable energy supply and cost-effective scalability. However, substantial work is required to find suitable electrocatalysts to facilitate the stubborn CO_2 reduction process. Metal-organic frameworks (MOFs) have obtained interest in the application of electrocatalysis. The interest arises from innate features of MOFs including permanent porosity, high surface areas, and versatility. Although various MOF structures have been utilised in the electrochemical CO2 reduction reaction (CO2RR), two particular limitations hinder the electrocatalytic performance. [1]

The first limitation arises from the electrochemical cell design commonly used in electrocatalysis. Typically, CO_2 is dissolved in solution-phase and diffuses to the electrocatalyst. The solubility limit (34 mmol/L) and slow diffusion kinetics of aqueous CO_2 hinder the mass transport of CO_2 resulting in generally low conversion rates.[2]

The second limitation arises from the typical resistivity nature of MOFs. The charge transport capabilities of electrocatalysts are a significant contributor to the CO_2 conversion rate. MOF materials are typically quite insulating (10^-10 S/cm) which arises from poor overlap between metal node and organic linker molecular orbitals.[3]

To overcome the limitations of MOF-based CO_2RR electrocatalysis, we utilise a gas diffusion electrochemical cell, which provides a short and quick diffusion path to the electrocatalyst thereby enhancing mass transport. To overcome poor electrical conductivity, we implant conductive polymer species within the pores of a MOF thereby enhancing charge transport.

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Immobilized Molecular Catalysts for Heterogeneous Electrochemical Hydrogen Evolution (HER) and CO2 Reduction (CO2RR)

Mr Kieran Demonte[1,2], Prof. Sally Brooker, Prof. Aaron Marshall
[1]University Of Otago, Dunedin, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand, [3]University of Canterbury, Christchurch, New Zealand

Session 11A: CO2 reduction, Auditorium, February 13, 2025, 14:25 - 16:00

The global use of fossil fuels results in unsustainable levels of CO_2 gas being released into the atmosphere, furthering the impacts of global warming.[1] Possible capture of CO_2 from high emission processes and subsequent selective reduction (CO_2 reduction reaction, CO_2RR) to convert it into renewable fuels could move those processes towards carbon neutrality.

To move towards carbon zero, green hydrogen is a desirable alternative to fossil fuels. Hydrogen has a higher energy density and only produces water as a waste product. 'Green' hydrogen is produced from water using renewable energy (hydrogen evolution reaction, HER). Most hydrogen produced currently, for use in industry, is 'grey' hydrogen made from fossil fuels in energy intensive and carbon emitting processes, so this must also be replaced by green hydrogen.

The HER and CO2RR are energy intensive processes so catalysts are needed to reduce the energy of these chemical processes, to make them more energy and cost efficient.[2] The CO_2RR is a process with many possible products, highlighting the need for catalysts that can not only reduce the energy required for reduction but also produce the desired useful products selectively.

We have prepared a range of porphyrin-like dimetallic macrocyclic complexes[3],[4] and these are now being tested for electrocatalytic activity for HER and CO_2RR. This testing is being carried out under heterogenous conditions, through immobilisation of the catalysts on solid supports. This presentation will cover the synthetic steps involved in producing these macrocyclic complexes and the results of the heterogeneous electrochemical HER and CO_2RR testing on selected complexes.

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Innovative Applications of Laser-Scribed Graphene

Dr Bicheng Zhu[1]
[1]University of Auckland, Auckland, New Zealand

Session 11B: Biosensors and electronics, Dobson 1, February 13, 2025, 14:25 - 16:00

Organic biosensors and bioelectronics have become essential tools for advancing point-of-care diagnostics and wearable technologies due to their flexibility, affordability, and electrochemical properties. Laser scribing (LS) is an emerging technology ideal for the one-step, controllable fabrication of micro/nanostructured graphene. We have developed numerous applications in biosensing and bioelectronics using laser-scribed graphene, ranging from disposable electrochemical sensors for metabolite and pathogen detection to epidermal energy storage devices and electrocatalysts.

A strategy towards biomimetic and transient polymer (bio)electronics

Professor Jadranka Travas-Sejdic[1]
[1]The University of Auckland, Auckland, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand

Session 11B: Biosensors and electronics, Dobson 1, February 13, 2025, 14:25 - 16:00

The field of bioelectronics involves the fascinating interplay between biology and human-made electronics. However, the difference in the physical nature of soft biological elements and rigid electronic materials calls for conductive and/or electroactive materials with added biomimetic properties that can bridge the gap. Soft electronics that utilizes organic conjugated polymers can bring many important features to bioelectronics. Amongst the many advantages of conjugated polymers, the ability to modulate the biocompatibility, solubility, functionality and mechanical properties through side-chain engineering can alleviate the issues of mechanical mismatch and provide a better interface between the electronics and biological elements. In this talk, I will focus on our recent progress in the molecular engineering of conjugated polymers with tunable biomimetic properties, such as biocompatibility, responsiveness, stretchability, self-healing and adhesion, and their applications. Also, I will present our recent progress in utilising similar approaches to achieve transience in polymer electronics.

Designed solar harvesting protein antenna for bioelectronics and biocatalysis

Dr Dominic Glover[1]
[1]University of New South Wales, Sydney, Australia

Session 11B: Biosensors and electronics, Dobson 1, February 13, 2025, 14:25 - 16:00

Electron transfer through protein assemblies is a fundamental process of life for the production and use of energy, such as photosynthesis that converts solar energy into chemical energy to power biocatalysis. Harnessing the ability of proteins to transfer energy may enable the creation of bioelectronic devices from sustainable and nontoxic materials. This presentation will describe several engineering approaches to create electron and proton conductive protein-based materials that can be used to harness and transfer energy to enzymes for biocatalysis. Conductive protein nanowires were fabricated by aligning a variety of metalloproteins, such as cytochrome c3 in proximity along a protein filament. The resulting individual nanowires were capable of efficient long-range electron transfer, with a conductivity of up to 6 S/cm. As an alternative to attaching metalloproteins to filaments, we also demonstrated that protein assemblies can be rendered electronically conductive through the direct incorporation of heme molecules. Photoexcitable porphyrin molecules such as chlorophyll b or zinc protoporphyrin IX can be incorporated into the filaments using a similar strategy, which enabled the creation of nano-antennae for solar energy harvesting. In addition to producing electrical current, the photoactive protein antennae were able to transfer electrons to enzymes aligned along the surface. These enzymes were shown to perform biocatalysis and reduce specific substrates when these functionalized antennae were exposed to light. Ultimately, the creation of metalloprotein nanowires with tailorable conductive properties will serve as a foundation for building bioelectronic devices that bridge the biotic-abiotic divide.

Copolymers of gelatin and conducting polymers for Transient Electronics

Miss Xin Sun[1,2]
[1]The University of Auckland, Auckland central, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand

Session 11B: Biosensors and electronics, Dobson 1, February 13, 2025, 14:25 - 16:00

As transient electronics continue to advance, the demand for new materials has given rise to the exploration of conducting polymer (CP)-based electronic materials. The big challenge lies in balancing conductivity while introducing controlled degradable properties into CP-based transient materials. In response to this, we present in this work a concept of using conducting polymers attached to an enzymatically biodegradable biopolymer to create transient polymer electronics materials. Specifically, poly(3-hexyl thiophene) (P3HT) is covalently grafted onto biopolymer gelatin, affording graft copolymer gelatin-graft-poly(3-hexyl thiophene) (termed Gel-g-P3HT). The thin films of Gel-g-P3HT that were produced by optimized processing solvent (THF/H2O cosolvent) showed enhanced π–π stacking domains of P3HT, resulting in semiconducting thin films with good electroactivity. Due to the presence of amide bonds in the gelatin backbone, Gel-g-P3HT underwent degradation over a period of 5 days, resulting in the formation of amphiphilic micellar nanoparticles that are biocompatible and nontoxic. The potential of these conductive and degradable graft copolymers was demonstrated in a pressure sensor. This research paves the way for developing biocompatible and enzymatically degradable polymer materials based on P3HT, enabling the next generation of transient polymer electronics for diverse applications, such as skin, implantable, and environmental electronics.

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High Precision Multiplexed Measurements of Insect Odorant Receptors Immobilised on Carbon Nanotube Field Effect Transistor Platforms

Miss Danica Fontein[1,2], Alireza Zare[1,2], Dr Colm Carraher[3], Kingsley Omeje[1,3], Professor Adam Micolich[4], Dr Natalie Plank[1,2]
[1]Victoria University of Wellington, Wellington, New Zealand, [2]The MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand, [3]The New Zealand Institute for Plant & Food Research Ltd, Auckland, New Zealand, [4]University of New South Wales, Sydney, Australia

Session 11B: Biosensors and electronics, Dobson 1, February 13, 2025, 14:25 - 16:00

Keywords: Insect Odorant Receptors; Carbon Nanotube Network FET; Electronic nose; Multiplexed biosensing.

Insects possess an extraordinary ability to detect and distinguish chemical signatures, relying on their evolved repertoire of odorant receptors (ORs) to navigate their environment and perform essential survival tasks. [1] Recent breakthroughs in precision molecular biology and nanoelectronics have enabled the integration of insect ORs with field-effect transistor (FET) platforms, creating bioelectronic sensors that convert biorecognition signals into electronic outputs. [2,3]

We present an optimised, passivated FET platform utilising carbon nanotube (CNTs) functionalised with insect ORs, delivering a highly sensitive, reliable, and robust approach for real-time analyte detection. Our multiplexed detection system enables the simultaneous measurement of all eight OR-CNTFET sensors in a single experiment with femtoampere resolution. This innovative approach provides critical insights into the sensing mechanisms of the insect olfactory system, vital to the development of future electronic nose technologies and biomedical sensors more broadly.

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Function-coordinated Electrocatalysts for Carbon Dioxide Reduction

Professor Yuhang Li[1]
[1]East China University of Science And Technology, Shanghai, China

Session 11C: Electrocatalysis, Dobson 2, February 13, 2025, 14:25 - 16:00

The electrochemical reduction of carbon dioxide enables the storage of intermittent renewable energy in the form of chemical bonds. Further progress is required in the electrocatalysts which facilitate the conversion chemistry. The functional coordination structures of the electrocatalysts have been regarded as important factors for the catalytic performance of carbon dioixde reduction.Our research is in the area of fundamental studies of functional materials and systems for electrosynthesis [1-5]. By using the oxygen-containing functional groups of water-soluble polymers, we have regulated the reaction microenvironment for catalyst synthesis, and created the cluster-sized catalysts with rich oxygen donors. We found out that this kind of metal oxide catalysts exhibited excellent activity and selectivity for carbon dioxide reduction. Further, we have proposed a strategy to improve catalyst stability for carbon dioxide reduction, that is, by enhancing the oxygen transfer processes in the micro-region of electrode/electrolyte interface. By optimizing the electrolyte formula to match the catalytic materials, the applicant promoted the stability of the oxygen-containing active sites in metal oxide catalysts, thus achieving a cathode energy efficiency of more than 75% at high current density for carbon dioxide reduction. Recently, we have proposed to couple the processes of cathode and anode reactions, and devised a redox-mediated electrocatalytic reactor. This reactor realized the efficient production of ethylene oxide from carbon dioxide with low energy input and high conversion rate.

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Nanoscale Structure−Activity Mapping of Electrocatalysts

Dr Cameron Bentley
[1]Monash University, Clayton, Australia

Session 11C: Electrocatalysis, Dobson 2, February 13, 2025, 14:25 - 16:00

All solid surfaces—from the simplest monocrystals to the most complex composite nanomaterials—possess some degree of heterogeneity but determining how surface structure affects electrode functional properties (e.g., catalytic activity, selectivity, stability etc.) can often be challenging using traditional “bulk” electrochemical techniques. Scanning electrochemical cell microscopy (SECCM) is a nanopipette-based scanning probe microscopy (SPM) technique that utilises a mobile droplet cell to measure and visualise electrochemical (electrocatalytic) activity with high spatiotemporal resolution. This presentation will spotlight the use of SECCM for probing the electrocatalytic activity of nanomaterials on a commensurate scale to surface structural heterogeneities (i.e., nm–µm scale). It will be demonstrated that this approach is widely applicable to: well-defined monocrystals (e.g., transition metal dichalcogenides: MoS2 and WS2); structurally and/or compositionally heterogeneous polycrystals (e.g., polycrystalline Pt, Pd, Cu, etc) and; composite nanoparticle-on-support “ensemble” electrodes [e.g., β-Co(OH)2 nanoplatelets supported on carbon]. In particular, it will be emphasised how nanoscale-resolved information from SECCM is readily related to electrocatalyst structure and properties, collected at a commensurate scale with complementary, co-located microscopy/spectroscopy techniques (e.g., SEM, TEM, EBSD, AFM etc.), to allow structure−activity relationships to be assigned directly and unambiguously.

Oxygen Driven Defect Engineering of Monolayer MoS2 for Tunable Electronic, Optoelectronic, and Electrochemical Devices

Miss Sindhu Priya Giridhar[1], Dr Irfan H. Abidi, Prof Sumeet Walia
[1]RMIT University, Melbourne, Australia

Session 11C: Electrocatalysis, Dobson 2, February 13, 2025, 14:25 - 16:00

Aim:
Two-dimensional(2D) materials such as transition metal dichalcogenides(TMDs) are emerging as suitable alternative semiconducting material to the existing silicon-based electronics and optical technologies. The performance of TMDs such as monolayer MoS2 relies on the quality of 2D atomic crystals, which can be influenced by atomic defects such as sulfur vacancies(Vs) and atomic substitutions[1,2]. Achieving reliable and scalable defect engineering in monolayer MoS2 poses significant challenges. Usually requiring a two-step process that includes aggressive post-synthesis processing with detrimental effects on monolayer MoS2. This work demonstrates a simple, effective, and scalable strategy to inherently regulate the formation and/or the passivation of Vs defects on demand within monolayer MoS2, by tuning the pressure during chemical vapour deposition(CVD) growth[3].

Method:
CVD was used to obtain monolayer MoS2 crystals in low pressure(LP) oxygen deficient and atmospheric pressure(AP) oxygen rich conditions[3]. Standard photolithography techniques were deployed for devising two terminal lateral devices[3].

Results:
LP CVD-grown MoS2(LP-MoS2) had Vs induced defect-rich crystals primarily attributed to the oxygen-deficient growth conditions. Conversely, AP CVD-grown MoS2(AP-MoS2) passivates these defects with oxygen from ambient conditions[3]. This disparity in defect profiles profoundly impacts functional properties and device performance. The n-doping induced in LP-MoS2 generates enhanced photoresponsivity and detectivity in fabricated photodetectors compared to the AP-MoS2-based devices[3]. Defect-rich LP-MoS2 outperforms AP-MoS2 as channel layers of field-effect transistors(FETs), as well as electrocatalytic material for hydrogen evolution reaction(HER)[3].

Conclusion:
We have demonstrated the effectiveness of our in-situ defect engineering strategy for customizing TMDs such as MoS2, for targeted applications in optoelectronics, electronics, and catalytic devices.

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Theoretical investigation and screening of dual-atom catalysts (DACs) for the oxygen reduction reaction

Dr Yu Mao[1], Dr Ziyun Wang[1], Professor Geoffrey Waterhouse[1]
[1]University of Auckland, Auckland, New Zealand

Session 11C: Electrocatalysis, Dobson 2, February 13, 2025, 14:25 - 16:00

The oxygen reduction reaction (ORR) plays a vital role in many next-generation energy storage devices, including proton-exchange membrane fuel cells (PEMFCs) and zinc-air batteries (ZABs). In recent years, metal single-atom catalysts (SACs), comprising atomically dispersed metals on N-doped carbon supports, have emerged as a promising alternative to expensive Pt/C catalysts for ORR. Dual atom catalysts (DACs), comprising atomically dispersed metal dimers, particularly those with heteronuclear metal sites, offer significant opportunities for boosting the kinetics of the oxygen reduction reaction. However, the rational design of efficient DACs for the ORR remains largely unexplored and challenging. Herein, I will discuss our recent research aimed at the computational screening of DACs for ORR, seeking to combine the benefits of single-atom catalysts and metal alloy nanoparticles. Large-scale density functional theory (DFT) screenings were employed to explore the *O-*O scission mechanism, which can circumvent the traditional scaling relationships that limit ORR activity, thus explaining the superior catalytic performance of N-doped graphene-supported Fe-, Co-, Ni-, and Cu-containing heteronuclear dual-atom catalysts. New dual-atom catalysts were found to possess high activities and outperform the best single-atom catalysts. The chemical and structural basis of the *O-*O scission mechanism, thus leading to enhanced reaction activity over DACS, has been revealed. This work not only provides additional insights into the fundamentals of the ORR but also offers guides for the accelerated discovery of efficient dual-atom catalysts.

Oxygen bubble formation under confinement

Miss Ghazaleh Ramezani[1], Dr Kim Mckelvey[1], Marissa Dierkes[1], Jaimy Monteiro[1]
[1]Victoria University of Wellington, School of Chemical and Physical Sciences, Wellington, New Zealand, ,

Session 11C: Electrocatalysis, Dobson 2, February 13, 2025, 14:25 - 16:00

Green hydrogen production via water electrolysis relies heavily on electricity, making the improvement of energy-efficient water electrolyzers crucial for the future hydrogen economy. Newly developed Anion Exchange Membrane Water Electrolyzers (AEMWELs) offer significant cost reductions through the use of inexpensive and abundant electrocatalysts, as well as low-cost membranes.1

A significant challenge associated with AEMWELs is the formation of oxygen (O_2) bubbles on the anodic electrode surface. The attachment of bubbles reduces the contact area between the electrode surface and the liquid phase, resulting in a decreased effective electrochemical reaction area, which impacts the electrode performance. This problem is exacerbated by the use of highly porous electrodes, which can lead to the formation of O_2 nanobubbles between the catalyst particles.2

We quantify the formation and behavior of O_2 nanobubbles produced during the anodic oxygen evolution reaction(OER) on a Ni electrocatalyst in a nanoconfined environment using a meticulously lithography-patterned nanofluidic channel. We are able to measure the instant of nanobubble formation. This provides insights into the precise generation sites and concentrations of O_2 nanobubbles formed during the OER. Our findings have implications for the design of OER electrocatalysts.

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Changing Metals and Their Atoms On by One in Subnanometer Clusters and Switching Supports to Control Catalytic Activity and Selectivity

Dr Štefan Vajda[1]
[1] J Heyrovsky Institute of Physical Chemistry, Czech Academy of Sciences, Prague, Czech Republic

Session 11D: Nanoparticles, Dobson 3, February 13, 2025, 14:25 - 16:00

The presentation will report on how the cluster size, atomic composition in bimetallic particles and cluster-support interaction can be used to control catalyst performance from switching selectivity up to boosting activity by orders of magnitude. The approach will be demonstrated on the examples of oxidative and non-oxidative dehydrogenation of cyclohexene sing oxide and carbon-supported The example of oxidative dehydrogenation of cyclohexene where an atomic precision mono- and bimetallic clusters made of a handful of atoms, such as Cu, Pd and CuPd custers.

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Molecular effects for tuning charge transport in nanostructured hybrid materials

Dr Simon Tricard[1]
[1]LPCNO, CNRS, INSA, Université De Toulouse, Toulouse, France

Session 11D: Nanoparticles, Dobson 3, February 13, 2025, 14:25 - 16:00

A main goal of molecular electronics is to relate the performance of devices to the structure and electronic state of molecules. Electronic measurements through nanoparticle (NP) self-assemblies (SA) show that charge transport is dominated by tunneling or co-tunneling mechanisms. In such NP SAs, charging energy is the energy cost that has to be paid to put an additional electron on a NP. The charging energy creates a Coulomb energy gap, which suppresses low-bias conduction in the effect called Coulomb blockade.

The goal of the presented work is to develop SAs between ultra-small Pt NPs and functional molecules. Tuning the strength of the coordination interactions between the molecules and the NP surface allowed to control the structure of the SAs. Another originality of our approach is to consider the intrinsic physicochemical characteristics of the molecules between the NPs and not to simply see them as a continuous dielectric medium. Three main results will be presented. 1) When Pt NPs are sufficiently small (< 2 nm), Coulomb blockade is present at room temperature, which is of particular interest to facilitate experiments. 2) The use of a series of polyoxometalates made it possible to prove that polarizability is an essential parameter to rationalize electrical measurements involving molecules. This new conceptual approach for considering molecular response in NP SA gives new opportunities in molecular electronics. 3) Using a coordination polymer, the polarizability of which changes with spin crossover, we were able to tune charge transport by an internal switch in temperature.

Catalytic activities of waste-derived gold nanoparticles

Miss Michelle Lau[1], Dr David Young[2], Dr Jack Chen[3], Professor Johnathan Sperry[4]
[1]University Of Auckland, Auckland, New Zealand, [2]Mint Innovation, Auckland, New Zealand, [3]School of Chemical, Auckland University of Technology, [4]Centre for Green Chemical Science, University of Auckland, New Zealand

Session 11D: Nanoparticles, Dobson 3, February 13, 2025, 14:25 - 16:00

Typical methods to produce gold nanoparticles (AuNPs) utilise solutions containing 1000 to 27 000 ppm of gold.1–3 These precursor solutions are derived from purified raw ore materials and are not representative of waste-derived solutions that typically range from 20 to 30 ppm.4 Electronic waste (e-waste) is a growing concern worldwide, due to the presence of various toxic substances that can leach into the environment and threaten human health.5 However, e-waste is a rich source of precious metals including Au, Pd, and Ag, which brings to focus the creation of a circular economy for generating value-added products from waste.5 AuNPs derived from e-waste have been previously reported, but their corresponding catalytic function has never been evaluated or optimised.6–8 This research discusses the synthesis of AuNPs derived from solutions at concentrations representative of e-waste leachates. These AuNPs are further evaluated and optimised for their catalytic utility for organic syntheses and are subsequently compared against real-life e-waste-derived AuNP samples.

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Ultra-Small Gold Nanoparticle Particle Adsorption and Uptake is Directed by Particle Capping Agent

Dr Aaron Elbourne[1]
[1]Rmit University, Melbourne, Australia

Session 11D: Nanoparticles, Dobson 3, February 13, 2025, 14:25 - 16:00

Introduction: Nanomaterials are widely investigated, especially in many biological settings. This is due to their potential use as advanced nano-medicines and diagnostic technologies. In general, nanoparticle-based biotechnologies must interact with, and often cross, a cellular membrane to be useful; however, the dynamics of these interactions are still poorly characterized.

Aim: Combine advanced experimental and computational studies to investigate the interaction of ultra-small gold nanoparticles (AuNPs) with a variety of systematically varied capping agents at the interface of synthetic bio-membranes to determine the dynamic interaction of model systems at bio-membranes.

Methods: A combination of atomic force microscopy, light and energy scattering, and molecular dynamics simulations was used to study the fundamental behavior of the AuNPs at the bio-membrane-liquid interface. The systems of interest are models consisting of supported lipid bilayers (SLBs) and free-floating liposomes, which act as archetypal bio-membranes. The capping agent on the particles was purposefully varied. Liquid-phase and gel-phase biomembranes were used to systematically assess interactions.

Results: We investigated the behavior—dynamics, adsorption, translocation, and physical interactions—of a variety of AuNPs at the biomembrane interface. The techniques listed above are beginning to provide localized, nanoscale information on the dynamics and mechanisms governing the interactions of AuNPs and biomembranes.

Conclusion: The precise mechanism by which AuNPs adsorb to the bio-membrane is beginning to be elucidated, revealing several interesting behaviors: 1) initial adsorption, 2) nanoparticle incorporation and/or translocation, 3) particle-induced phase change, and 4) translocation of the particles. These interactions are of broad scientific and medical interest.

Improving the memory of percolating networks of nanoparticles

Mr Ben Monaghan[1], Mrs Sofie Studholme[1], Professor Simon Brown[1]
[1]University Of Canterbury, Christchurch, New Zealand

Session 11D: Nanoparticles, Dobson 3, February 13, 2025, 14:25 - 16:00

Novel brain-inspired computer architectures have been proposed as alternatives to the conventional von Neumann architecture with the aim of emulating the low power demands and aptitude for certain tasks of the human brain. Self-organised percolating networks of nanoparticles (PNNs) operating in low-voltage regimes have been shown to act as networks of memristors for use in reservoir computing (RC) applications [1] but lack the dynamics of criticality displayed in higher-voltage 'switching' regimes [2]. The aim of this project is to simultaneously exploit both advantages by replacing some spiking tunnel gaps in switching-regime PNNs with memristors, with our hypothesis being that these mixed-type networks may display both critical dynamics and RC aptitude. These mixed-type PNNs are being simulated with a generic memristor model for the replaced tunnel gaps, and a key focus of the project has been whether they maintain both critical dynamics and the desired properties of the low-voltage PNNs. We demonstrate that networks predominated by switching gaps with a small proportion (less than 40%) of gaps replaced by memristors have a unique relationship with the desired critical dynamics, while networks predominated by memristors show no evidence of criticality.

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Why is gallium liquid at room temperature*?

Professor Nicola Gaston[1]
[1]The MacDiarmid Institute for Advanced Materials and Nanotechnology, Auckland, New Zealand

Session 11E: Modelling and materials theory, Dobson 4, February 13, 2025, 14:25 - 16:00

The use of low-temperature liquid metals, such as gallium, as media for the dilution of other metals has led to an increasing variety of examples of how temperature- and concentration-dependent interactions can be used to direct the self-assembly of nanostructure, with astonishing precision, resulting in novel pattern formation and structural control. However the underlying interactions driving such phenomena are still poorly understood.

A question of fundamental importance remains to be answered: why does gallium have such a low melting temperature, of 29.8 degrees Celsius, to begin with?

Recent first-principles simulations have demonstrated that, in contrast to previous assumptions, covalent bonding becomes more important in the liquid at higher temperatures, meaning that covalency is not a significant feature of the liquid near the phase transition temperature. This explains the experimental observation of a decrease of resistivity of the metal upon melting, and its subsequent anomalously nonlinear increase with temperature.

It also suggests that the change of enthalpy upon the change from solid to liquid phase is not anomalous, and that instead the entropy difference between the dimeric solid and monatomic liquid explains the room temperature (on a nice day) melting point [1].

*The mean daily maximum air temperature in Christchurch, in February, is apparently 22.2 degrees Celsius. Please excuse the poetic license and imagine that we leave it to sit in the sun for a bit!

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Modelling surface solidification of binary alloys with a phase-field Lattice Boltzmann model

Dr Alexander Smith[1,3], Dr Krista Steenbergen[2,3], Prof Nicola Gaston[1,3]
[1]The University of Auckland, Auckland, New Zealand, [2]Victoria University of Wellington, Wellington, New Zealand, [3]The MacDiarmid Institute of Advanced Materials and Nanotechnology, Wellington, New Zealand

Session 11E: Modelling and materials theory, Dobson 4, February 13, 2025, 14:25 - 16:00

Eutectic surface solidification in binary alloys offers a unique pathway for tuning the growth of nanostructures to optimise their mechanical, optical, and catalytic properties. While bulk solidification processes are well-characterized, the ability to precisely control surface solidification remains underexplored. Understanding and harnessing the mechanisms of surface solidification in binary alloys, especially in relation to imposed cooling rates and composition, could open new avenues for engineering nanostructured surfaces with properties optimised for next-generation technologies.

Motivated by recent experimental work that observes the formation of highly-ordered surface structures during the solidification of Bi-Ga alloys [1], a hybrid computational approach using the Lattice Boltzmann Method (LBM) in conjunction with a phase-field model [2, 3] has been developed to investigate the underlying mechanisms relevant to controlling surface solidification and designing tunable nanostructures. By integrating the LBM's capability to model complex flow and transport phenomena with the phase-field approach's strength in tracking evolving interfaces, this method provides a powerful tool for predicting and optimizing the formation of nanoscale structures with high spatial and temporal resolution.

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High-throughput Predictions of Impact Ionization Properties for Material Discovery

Mr Ryan Hall[1], Dr Fiacre Rougieux, Prof. Francois Ladouceur, Mr Norbert Krause
[1]University Of New South Wales, Sydney, Australia

Session 11E: Modelling and materials theory, Dobson 4, February 13, 2025, 14:25 - 16:00

Impact Ionization plays a critical role in a wide range of devices, including avalanche photodiodes, LEDs, power transistors and MOSFETs. Carrier generation by Impact ionization is also used in the contacts of emerging wide bandgap optoelectronic devices [1] to efficiently inject carriers, mitigating the doping challenges associated with conventional wide bandgap material systems and unlocking applications for new and existing materials that might have previously been deemed unsuitable for semiconductor devices due to doping limitations.

The impact ionisation scattering rate is a critical parameter in the search for novel wide-bandgap materials. However, current impact ionization models can be poorly predictive, often assuming a parabolic band dispersion relation or failing to take advantage of recent advances in ab-initio electronic structure calculations. On the other hand, advanced models require the calculation of the transition matrix elements which comes at an immense computational cost, precluding high-throughput studies for material screening and prediction.

For high-throughput material screening, there is a critical need for a fast and accurate model for the impact ionisation scattering rate. In this study, we bridge this critical gap and develop a high-throughput computational method to calculate the impact ionization threshold as a function of the primary carrier momentum and from this, the energy-dependent probability of impact ionization for ultra-wide bandgap semiconductors. We arrive at a computationally efficient first-principles estimation of the impact ionization scattering rate by using the aforementioned properties to compute a momentum-dependent modification to Kane's rate [2] that is consistent with experimental findings in the literature. We utilise the pre-computed DFT electronic structure calculations of tens of thousands of materials hosted by the Materials Project database [3] to enable a high-throughput study.

We find that the impact ionization thresholds and scattering rates computed in this work are consistent with measurements in the literature and show that the impact ionization threshold energy alone is a suitable low-cost estimator of the more computationally expensive full scattering rate. We use our methods to calculate energy-dependent impact ionization scattering rates for several conventional ultrawide bandgap material systems including GaN, AlN, β-Ga2O3 and MgO and show a range of interesting asymmetry in electron/hole impact ionisation rates in both existing and unexplored material systems that could be exploited in the design of optoelectronic devices.

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Poster Presentations

Immobilization and Catalytic Conversion of Polysulfides by In-Situ Generated Nickel in Hollow Carbon Nanofibers for High Performance Lithium–Sulfur Batteries

Professor Jou-Hyeon Ahn[1], Professor Soonho Hwangbo[1]
[1]Gyeongsang National University, Jinju, South Korea

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Lithium-sulfur (Li-S) batteries are considered promising energy-storage systems because of their high theoretical energy density, low cost, and eco-friendliness. However, serious problems, especially the notorious shuttle effect, can result in the loss of active material, poor cyclability, and rapid capacity fading. The utilization of a structural configuration that enhances the electrochemical performance via adsorption-catalysis dual strategies can overcome the limitations of Li-S batteries. Herein, an integrated interlayer structure, in which hollow carbon fibers (HCFs) were modified with in situ generated nickel (Ni) nanoparticles, was prepared by a scalable one-step carbonization method. Highly conductive and hierarchically porous HCFs as the carbon skeleton provide a continuous three-dimensional (3D) conductive network to enhance the ion/electron diffusion and physically confine polysulfide diffusion. The Ni nanoparticles with superior anchoring ability and a strong catalytic effect can prevent the shuttle effect and increase the conversion rate of polysulfides, promoting excellent electrochemical performance at high rates. This synergistic effect resulted in a high capacity retention of 582 mAh/g at 1 C after 100 cycles, providing an excellent rate capability of up to a 3 C. The novel structure wherein Ni nanoparticles are embedded in cotton-tissue-derived HCFs provides a new avenue for enhancing the electrochemical performance at high C rates, affording a low-cost, sustainable, high-performance hybrid material for the development of practical Li-S batteries.

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Elucidating Ca2+ and H2O2 Signalling in Plant Roots: Responses to Osmotic Stress, PAMPs and Force Sensing Using Linear Treatment Gradients

Ms Claudia Allan[1], Yiling Sun[1], Haig Bishop[1], Claudia-Nicole Meisrimler[1], Volker Nock[1]
[1]The University of Canterbury, Christchurch, New Zealand

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Signal transduction in plants is essential for detecting and responding to environmental stress, with Ca2+ and reactive oxygen species (ROS) playing pivotal roles [1]. However, the mechanisms regulating adaptation during osmotic and pathogen stress are unclear. Microfluidic platforms, including the bi-directional-dual-flow-RootChip (bi-dfRC) facilitate the culture of plants containing fluorescent detectors, guide growth and expose roots to asymmetric solute gradients [2,3,4]. Here, the platform also utilises force sensing technology with displaceable micropillars to monitor root extension and growth force responses. We observed distinct directional Ca2+ signals and localised H2O2 accumulation in response to asymmetrically perfused osmolytes (NaCl, PEG) and pathogen-associated molecular patterns (PAMPs), including flg22 and Pep-13. Signal dispersion varied based on treatment and orientation, demonstrating directional responses. When osmolytes or peptides were applied at the shoot site, a concentration-dependent Ca2+ burst initiated at the differentiation zone (DZ) and rapidly traversed from the contact to non-contact site of the root, followed by a secondary signal dispersing tip-ward. Conversely, when stressors were applied at the tip site, a strong Ca2+ signal was observed at the tip. H2O2 accumulation occurred at cells in direct contact with the stressor, exhibiting localised upregulation over time. Additionally, pillar displacement revealed that the force exerted by multi-celled A. thaliana root tips significantly increased, and roots responded to force with a strong directional Ca2+ signal initiating at the elongation zone. This research aims to enhance understanding of plant sensing and response mechanisms, potentially contributing to the development of crops with improved tolerance to diverse stresses and pathogens.

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Optimizing UHPFRC Mixtures with Nano-Kaolin Clay and Steel Fibers for Improving 3D Concrete Printing Performance

Dr Fadi Althoey[1]
[1]Department of Civil Engineering, College of Engineering, Najran University, Najran, Saudi Arabia

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Ultra-high-performance fiber-reinforced concrete (UHPFRC) is increasingly utilized in advanced construction techniques, such as 3D concrete printing (3DCP), due to its superior properties. This study investigates the impact of integrating recyclable and reconfigurable materials, specifically nano-kaolin clay (NKC) and double-hooked end steel fibers (DHE-SFs), on the fresh and hardened properties of UHPFRC mixtures. This research supports the development of advanced materials for the circular economy, promoting sustainable construction practices. A series of rheological tests, including flowability, viscosity, and yield stress, were conducted along with pumpability and buildability trials at various print speeds. Results indicate that adding NKC and DHE-SFs to UHPFRC mixtures affects their workability and structural integrity. While initial flowability decreases, post-flow table drops show increases between 17.1% and 32.5%, balancing cohesiveness and workability for effective 3DCP. The presence of NKC and DHE-SFs significantly influences viscosity, with shear-thinning behavior and viscosity increasing up to 145.7% in mixtures with higher fiber and nanoparticle content. This adjustment in rheological properties is crucial for maintaining the mixture's shape stability and structural integrity during printing. The study also reveals that NKC and DHE-SFs enhance yield stress, with mixtures having 3% fibers and 0.5% NKC, achieving the highest initial yield stress, indicating superior shape retention necessary for 3DCP. Pumpability trials confirm that mixtures with higher NKC and DHE-SFs maintain pumpability at higher speeds, and buildability trials show these mixtures retain structural integrity without collapsing. Hardened property tests demonstrate significant improvements in compressive and tensile strengths, with mixtures achieving up to 150 MPa in compressive strength and 12 MPa in tensile strength. These findings highlight the potential of NKC and DHE-SFs to optimize UHPFRC for 3DCP applications. By incorporating recyclable and reconfigurable materials, this research advances the circular economy, enhancing durability and performance in sustainable construction.

Towards the Development of a Novel Electrochemical Sensor for the On-Site Detection of Illicit Drugs

Ms Elise Bailey[1,2,3], Dr Lisa I. Pilkington[1,3], Prof. David Barker[1,2]
[1]School of Chemical Sciences, The University of Auckland, Auckland, New Zealand, [2]The MacDiarmid Institute, Wellington, New Zealand, [3]Te Punaha Matatini, Auckland, New Zealand

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Rapid, on-site sensors for the detection of illicit drugs in complex samples are of significant research and law-enforcement interest. We have identified three major areas of sensor need: detection of substances commonly used in drug-facilitated sexual assault, detection of illicit substances in samples collected from individuals requiring drug tests (e.g. roadside drug testing), and detection of potentially hazardous cutting agents in recreational drugs.

Conducting polymers have been shown to provide a promising sensing platform across a range of targets. Their unique electrochemical properties mean that any changes to the system can be investigated electrochemically, and thus upon functionalization and subsequent attachment the analysis of virtually any analyte of interest is possible.

Recently, our research group has developed a system using thiol-functionalized poly-3,4-ethylenedioxythiophene (PEDOT) for sensing a range of analytes via disulfide bond formation, from small molecules to biological entities, but this has not been used for forensic applications, nor in the general detection of drugs.(1,2)

This project involves the synthesis of thiol-functionalized thiophene monomers, and extensive characterization of the corresponding conducting polymers. These polymers form the basis of an electrochemical detection system for illicit substances that is capable of sensing in complex liquid samples.

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The Development of a Harakeke (Phormium tenax) Membrane Towards Sustainable Water Purification.

MX Jaye Barclay[1]
[1]Victoria University of Wellington, Wellington, New Zealand

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Membrane processes are effective tools for water purification because they achieve continuous separation under mild conditions, have easy scalability of operations, high compatibility with other filtration methods, and adaptable properties to suit a variety of applications [1,2]. The majority of water filtration membranes are fabricated from artificial polymer materials [3]. However, these membranes are energetically and chemically intensive to fabricate, and are non-biodegradable once the end of their useful life is reached [4]. The production and disposal of polymeric membranes thus induces significant environmental impact. Recently, alternative organic materials such as graphene, chitosan, and wood have been increasingly investigated as sustainable alternative membrane materials for water purification. Plant materials such as wood are renewable, naturally porous materials that have exhibited an intrinsic affinity for filtering contaminants from water. However, consistent harvest of wood sections is not always feasible or accessible for consistent drinking water purification, and membrane performance is strongly influenced by the type of tree that wood is harvested from [5]. Harakeke is a taonga (treasure) species endemic to Aotearoa (New Zealand) of great cultural significance to Māori. Its leaves contain robust fibre and possess an intrinsically porous structure that bears striking resemblance to that of polymeric membranes. This research endeavours to develop a membrane for purifying drinking water from harakeke leaf tissues. Utilising Kaupapa Māori methodologies, this project will produce an environmentally sustainable, accessible tool for purifying household drinking water in a culturally synergistic and respectful fashion.

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Where is My Capsule?

Miss Farzaneh Baserisalehi[1], Prof Volker Nock[1], Associate. Prof Ebu Avci[1]
[1]University Of Canterbury, Christchurch, New Zealand

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Smart capsules are used for the purposes of diagnosis and treatment in the gastrointestinal tract via sensing, sampling, drug delivery, and surgical operations including tumor removal [1, 2]. For their efficient operation, an accurate knowledge of the real-time capsule location in the gut is required. Therefore, multiple sensing methods have been suggested, such as magnetic, radio frequency-based, and visual tracking [3]. However, a method of capsule positioning with less error, the latter possibly due to body's tissues and fluids affecting electromagnetic signals (in the cases of magnetic and radio frequency sensing), and more precision, can make to-the-point diagnosis and treatment more reliable, safer, and overall, a game changer. Our proposed approach employs a merged sensing system combining pH and distance measurements to achieve confirmed positioning for an electrochemical capsule in the small bowel. The method begins with a miniaturised pH sensing module embedded in a fabricated capsule to determine the entrance of the robot from stomach to small intestine due to the distinct change in the pH level [4]. Once there, a remotely activated wheel will be pushed out of the capsule to roll against the intestinal wall to track the capsule via measuring its travelled distance by an integrated magnetic rotary encoder. Comparatively, no external sensor array and reference tracking object would be required to be attached to the subject since relative movement is considered [5]. The proposed method enables the capsule to be accurately navigated toward the point/s prescribed by diagnosis and treatment goals.

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Power dissipation for 2D and 3D percolating networks of nanoparticles (PNNs)

Professor Phil Bones[1], Dr Zachary Heywood[1], Dr Joshua Mallinson[1], Dr Matthew Arnold[2], Dr Simon Brown[1]
[1]University Of Canterbury, Christchurch, New Zealand, [2]University of Technology Sydney, , Australia

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

The interest in neuromorphic computing devices, which include PNNs, nanowire networks and arrays of memristors, is in part because they can operate at very low power [1, 2]. This work seeks to investigate by simulation whether that advantage, demonstrated already for two-dimensional PNNs [3], also applies to hypothetical three-dimensional PNNs.

In order to make the comparison, it is necessary to use a size metric for the two types of network; as a starting point, we have used the total number of particles deposited. We assume that both 2D and 3D PNNs can be modeled by continuum percolation theory.

At the largest sizes we have simulated, the network conductance for devices with deposition halted at 95% of the percolation threshold is approximately 0.008 S for 2D and is approximately 0.3 S for 3D. For comparison purposes, we assume that a voltage of 1 V is applied to 2D devices, whereas a lower voltage of 0.5 V is applied to 3D devices (corresponding to the difference in the mean lengths for dominant current paths in the 2D and 3D networks) [4]. The results to date suggest that dissipating the amount of heat generated internally may be significantly more difficult for 3D PNNs than for 2D PNNs.

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Developing Novel Lanthanide Framework Materials for CO2 Uptake and Catalysis

Mr Yichao Cai[1]
[1]Aut, Auckland, New Zealand

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With increasing populations and industrialization, meeting our climate and sustainability goals regarding the increased carbon dioxide (CO_2) emissions will require not only the further development of CO_2 capturing technologies, but also increasing technologies that can convert CO_2 to useful materials. One key transformation is the cycloaddition reaction of epoxides to form cyclic carbonates by inserting CO_2, a reaction where the rate can be increased in the presence of a Lewis acid catalyst. Lanthanide-based coordination polymers have proved to be promising candidates for the development of CO_2 cycloaddition catalysts, and herein, the use of two ligands systems (1,8-naphthalimide-sulfonate ligands and 1,2,3-triazole ligands with carboxylic groups) and their lanthanide-based coordination polymers for the development of multifunctional CO_2 activation catalysts is presented. Surface attachment of catalysts is an important area of research, and with our highly modular systems (1,2,3-triazole click chemistry) we can incorporate surface attachment substituents with relative ease. Our investigations into the surface attachment of our lanthanide (3+) coordination compounds for developing heterogeneous catalysts coatings will also be presented.

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Construction of a Z-Scheme Heterojunction for Next-Generation Photovoltaic Devices

Ms Jodi Carter[3], Dr Nathaniel Davis[3]
[1]Victoria University of Wellington, Wellington, New Zealand, [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand, [3]Dodd-Walls Centre for Photonic and Quantum Technologies, Dunedin, New Zealand

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Photovoltaic technologies have significant potential in combating climate change, but they currently only efficiently capture a limited portion of the solar spectrum. These inefficiencies stem from the interaction of photons with semiconductors, resulting in transmission and thermalization losses. Various approaches, such as multiple exciton generation, singlet fission, and triplet-triplet annihilation upconversion, have been explored to enhance the harvesting of the solar spectrum, but none have yet reached commercialization. Here, we propose the construction and characterization of a Z-Scheme heterojunction using two inorganic semiconductors for upconversion in solar cells. This upconversion process occurs when each semiconductor absorbs a low-energy photon, facilitating electron-hole recombination and allowing the remaining free charges to be extracted. This results in an "upconverted energy," enabling a low bandgap device to produce higher voltages. This allows the remaining free charges to be extracted, obtaining an 'upconverted energy'.

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Contact Angle Experiments for resin 3D Printing vs PMMA Micro-Milling - ELISA Lab-On-A-Chip Development

Miss Alice Cerdeira[1], Miss Milan Hildreth[1], Dr Azadeh Hashemi[1], A/Prof Deborah Munro[1]
[1]University of Canterbury, Christchurch, New Zealand

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Microfluidics is a rapidly advancing field with a wide range of applications across various industries, especially medical diagnostics, drug development, and screening[1]. Point-of-care (POC) devices utilising microfluidics enable rapid, on-site medical diagnostics, and these functions can be combined and streamlined onto a single chip, creating a system known as lab-on-a-chip (LOC)[2]. By leveraging microscale fluid mechanics, LOC miniaturises and accelerates assays, enabling POC applications that speed up and improve patient outcomes[3]. The focus of this research project has been the development of an ELISA (Enzyme-Linked Immunosorbent Assay)-based LOC (Figure 1) using two substrate materials, 3D printed resin and micro-milled PMMA (polymethylmethacrylate).

An ELEGOO Saturn 4 Ultra resin 3D printer and a Datron Neo micro-mill with PMMA sheets were compared for suitability in LOC applications. After fabrication, plasma ashing was necessary to create hydrophilic surfaces, and both substrates yielded comparable results. However, the practicality of plasma ashing for POC devices is limited. Thus, using surfactants, specifically Tween20, was explored to induce hydrophilic interactions and facilitate capillary flow[4]. Testing results showed distinctly different behaviour between substrates, which was further explored using contact angle. Increasing Tween20 concentrations reduced the contact angle, shown in Figures 1 and 2, though at different rates for each material. However, by adjusting surfactant concentrations, it may be possible to standardise flow characteristics across different substrates, enhancing their versatility.

This research highlights the potential for interchangeable use of LOC substrate materials by fine-tuning surfactant interactions as another approach for the development of robust, adaptable point-of-care diagnostic devices.

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Photophysics of Luminescent Polyacene Metal Organic Frameworks

Mr Sanutep Chan[1,2,3], Miss Lara Browne[1,2,3], Mr Finnian Blaauw-Smith[1,2,3], Miss Edin Liu[1,2], Mr Shae Patel[1,2], Miss Aditi Kumar[1,2], Dr. Lujia Liu[1,2], Dr. Nathaniel Davis[1,2,3]
[1]Victoria University of Wellington, Wellington, New Zealand, [2]The Alan MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand, [3]The Dodd-Walls Centre for Photonic and Quantum Technologies, Dunedin, New Zealand

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Energy transfer between luminophores – fluorescent species – depends on the distance between them and their spatial alignment (anisotropy). The commonly accepted exchange pathways are: Resonance interactions of molecular dipoles – Fluorescence Resonance Energy Transfer - and electron transfers – Dexter Electron Transfer. In the solution phase the luminophores are typically randomly oriented and diffuse giving an ever changing spread of energy transfer enabled and disabled microstates.

Metal organic frameworks are polycrystalline materials composed of metal ion clusters and organic molecule linkers. The high degree of order gives directed arrangements of the monomers in space. This characteristic can be exploited for energy transfer purposes, giving forced luminophore orientations and distances.

A series of luminescent polyacene monomers were synthesised and subsequent metal organic frameworks constructed from them. The photophysical characteristics of the resulting materials were investigated and compared to one another.

Perovskite precursor mixing and dispensing using PDMS based microfluidic channels

Dr Linda Chen[1]
[1]Electrical and Computer Engineering, University of Canterbury, Christchurch, New Zealand

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Perovskite solar cells are gaining attention for their low-cost fabrication compared to traditional silicon solar cells. The thin film critical for photon absorption is typically deposited using a spin coating technique with an anti-solvent method which involves manual handling of the precursor and anti-solvent dispensing, that can lead to handling errors in the fabrication process, resulting in lor reproducibility.

One proposed solution is to use a syringe pump with the spin coater to automate the dispensing process. However, the moisture sensitivity of perovskite thin films requires fabrication to be done in a controlled atmosphere, often in a glove box. Adding syringe pumps to the limited space in a glove box can be challenging.

This research explores the development of a microfluidic-based solution mixing device that can combine mixing and dispensing of the precursor and anti-solvent for perovskite thin film formation. This device could be attached to the spin coater lid, saving space in the glove box and simplifying the fabrication process. The precise and repeatable dispensing provided by the microfluidic device could also facilitate the scaling up and commercialization of perovskite solar cell production. Ultimately, this innovation aims to improve the efficiency and reliability of perovskite solar cell fabrication.

In-situ Characterization of WS2 and GaN/WS2 Heterostructure by Reflection High-Energy Electron Diffraction

Mr. Po-Yen Chen[1], Mr. Ray-Yu Hong[1], Professor Ing-Song Yu[1]
[1]National Dong Hwa University, Hualien, Taiwan

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Reflection High-Energy Electron Diffraction (RHEED) is a powerful technique employed to characterize the surface of crystalline materials, which is also an analytical tool for the growth of thin films during the process of molecular beam epitaxy (MBE). Two-dimensional tungsten disulfide (WS2) and three-dimensional gallium nitride (GaN) are compound semiconductor materials with excellent physical and chemical properties. Moreover, the heterostructure of GaN and WS2 have been considered as a potential semiconductor for novel applications in electronics and optoelectronics. In this work, the annealing process in the ultra-high vacuum was executed for the 2D WS2 layer to enhance its crystallinity, and the surface condition of 2D WS2 layer was identified by the in-situ RHEED before and after heat treatment process. After achieving a higher-quality 2D WS2 layer, the growth of GaN thin films on 2D WS2 layer by MBE was carried out to obtain a GaN/WS2 heterostructure. During the formation of GaN/WS2 heterostructure, RHEED was used to investigate the surface and growth of GaN films. To confirm the structure of WS2 layers and GaN/WS2 heterostructure, the material characterization also included Raman spectroscopy, Scanning Electron Microscopy (SEM), Atomic Force Microscopy (AFM), X-ray Diffraction (XRD) and Transmission Electron Microscopy (TEM). In summary, the enhancement of crystal structure for 2D WS2 layer by annealing process and the formation of GaN/WS2 heterostructure have been investigated by the observation of in-situ RHEED images.

Potential in using CMUTs for particle manipulation

Dr Romain Arnal[1], Professor Volker Nock[1], Dr Gary Turner[1], Dr Linda Chen[1], Dr Joe Chen[1]
[1]University Of Canterbury, Christchurch, New Zealand

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Capacitive Micromachined Ultrasonic Transducers (CMUTs) are a relatively new kind of technology proving to be a cheaper, more versatile, and CMOS-compatible replacement to piezoelectric-based ultrasound transducers. These micromachined devices can be easily fabricated as 2D-arrays of individually controllable, high-frequency and high-bandwidth transducers enabling the manipulation of microscale objects such as cells and microparticles via acoustic streaming and acoustic radiation forces. Combined with microfluidics, CMUTs could assist in a wide range of uses such as in the alignment of cells, cell separation and cell transport. CMUTs are also ideal transducers for ultrasound imaging [1], photoacoustic imaging [2], localization microscopy [3] and various novel and state-of-the-art medical applications. We describe the fabrication and characterisation of CMUTs fabricated using the facilities offered in the University of Canterbury NanoLab and inspired by a polyCMUT design [4]. Lessons learned from fabrication will serve as a basis for developing novel CMUT designs and CMUT based-systems.

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UPWEARS – A EU Horizon project on sustainable e-textile solution for sportwear

Dr Yi Chen[1], Dr Marie Joo Le Guen[1], Elizaveta Graevskaya[1], Dr Sofiane Guessasma[2]
[1]Scion, Rotorua, New Zealand, [2]INRAE, Nantes, France

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Textile industry in Europe is facing significant challenges as it is one of the most polluting industries [1]. Both consumers and European regulations, are demanding more sustainable materials and manufacturing techniques. Electronic textile (E-textile), which combine the comfort of textiles with the functionality of flexible electronics, have emerged as a revolutionary solution for wearable applications [2]. In this context, UPWEARS (sustainable solutions for UPgraded smart WEARables and equipment in Sport) project, which was funded by EU Horizon in 2024, aims to build an innovative and replicable value chain from the valorisation of nature resources towards a bio-inspired e-textile for potential applications in sportwear. The project brings together 15 partners from seven countries, covering the entire technical e-textile value chain, from fibre to prototype manufacturing and testing. This includes fibre functionalisation, yarn and sensor production and integration, AI expertise as well as stakeholder engagement and market analysis. UPWEARS is also one of the first EU Horizon projects in which NZ organisation (represented by Scion) is participating since NZ became an associated country in Horizon Europe program since 2023.

In the first two years of UPWEARS project, we will focus on extracting natural fibres and lignin from biomass, such as flax, cork and hemp, and functionalising them to achieve tailored functions (electric conductive, hydrophobic and fire resistance). Environmentally friendly sensors will be developed based on these conductive natural materials and integrated with flexible fabrics for potential e-textile applications. This presentation will introduce the fundamental concepts, the planned workpackage approach and some preliminary results obtained so far.

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Carbon dioxide Captured by Amino Acids Containing Deep Eutectic Solvents

Mr Hung-Yi Chi[1]
[1]Department of Chemical Engineering, National Taiwan University, Taipei, Taiwan

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

This study explores CO_2 absorption by two deep eutectic solvents (DESs) containing amino acids using molecular dynamics (MD) simulations and quantum mechanics (QM) calculations. The DESs in question are a mixture of alanine (Ala) and lactic acid and a mixture of L-arginine (L-arg) and glycerol. MD simulations are employed to investigate physical absorption, while QM calculations are used to examine chemical absorption. Based on MD simulations, CO_2 preferentially interacts physically with the Ala DES compared to the L-arg DES. However, this result contradicts experimental reports [1,2]. According to QM calculations using density functional theory at the B3LYP/6-311G+(d,p) level and the solvation molecular density (SMD) continuum solvation model, both L-arg and Ala can form carbamates with a negative enthalpy. However, L-arg molecules have a negative Gibbs free energy, while Ala has a positive value, indicating that L-arg DES exhibits excellent carbon capture ability due to chemical absorption.

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Structural and Magnetic Phase Transitions in CoMoO4 and CuMoO4

Mr Jackson Fowler[1,2], Mr Joey Williamson[1], Prof. Grant Williams[2], Dr Shen Chong[1]
[1]Robinson Research Institute, Victoria University of Wellington, Lower Hutt, New Zealand, [2]School of Chemical and Physical Sciences, Victoria University of Wellington, Wellington, New Zealand

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Structural phase transitions can be induced in both cobalt and copper molybdate through the application of either temperature or pressure [1,2]. These transitions are associated with dramatic colour changes (purple→dark green and pale green→brown, respectively), which introduce numerous potential optical sensing opportunities. The particularly low pressures required to induce these phase changes (≤10 MPa) further enhance this applicability [3]. Investigation into the structural phase transition in $CuMoO_4$ has provided insight into the specific transitional mechanism of the compound. Utilising this insight, we have employed a post-synthesis air annealing process to stabilise the high-temperature phase (α-phase) of this compound and measure its unique low-temperature magnetic properties for the first time.

α-$CoMoO_4$ and γ-$CuMoO_4$, both in their low-temperature and high-pressure phases, undergo magnetic transitions into antiferromagnetically ordered states at 13 K and 1.75 K, respectively [4,5]. Increasing the applied magnetic field strength below these magnetic transition temperatures (TN) leads to further magnetic transitions, known as spin flops, as the field strength overcomes specific inter-atomic interactions within the crystal structures. In $CoMoO_4$, two spin flop transitions are observed that are unprecedentedly sharp and well-defined, occurring at 0.6 T and 3.8 T [4]. The identification of several possible super-super-exchange pathways, through which the antiferromagnetic order could be disrupted by the applied magnetic field, motivates neutron scattering measurements at different field strengths. We have been granted neutron beam time by ANSTO, which will provide insight into the nature of the antiferromagnetic state and how this ordered state evolves across the two spin flop transitions.

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Dopaminergic Janus Synapse on Neuroligin-2 Modified Gold-Coated Microspheres

Dr. Wonkyung Cho[1], Ms. Minji Jung[1], Professor Taek Dong Chung[1]
[1]Seoul National University, Seoul, South Korea

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Recent advancements in neural interface technologies have facilitated the direct integration of electronic devices with neurons, enabling chemical communication between biological and artificial systems. A promising technique in this field involves synaptogenesis, offering an opportunity for synaptic signaling between these systems. We reported the first successful formation of a Janus synapse between dopaminergic (DA) neurons and abiotic substrates using neuroligin-2 (NLG2) to induce synapse formation. Janus synapses were characterized by the use of synaptic cell adhesion molecules to construct interfaces, providing precise control over the signal location, direction, and neurotransmitter types involved, thus enabling targeted and multifaceted communication. In this presentation NLG2 is immobilized on gold-coated microspheres, which then initiate synaptogenesis upon contact with spatially isolated DA axons. The newly formed DA Janus synapses exhibit stable synaptic activity over time, similar to that of native synapses, indicating their potential for neural interface applications. The NLG2-immobilized abiotic substrates effectively promote the formation of DA presynaptic structures, making them a valuable tool for detecting chemical signals, dopamine release at the synapse level, and thus contributing to the progress of neural interface technologies.

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Unveiling Aggregation Propensity of Amyloid-β and Its Mutants Through Relaxation Dynamics

Parbati Biswas, Dr Priya Dey[1]
[1]iCeMS, Kyoto University, Kyoto, Japan

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Atomistic molecular dynamics simulations are employed to investigate the global and segmental relaxation dynamics of the amyloid-β protein and its causative and protective mutants. Amyloid-β exhibits significant global/local dynamics that span a broad range of length and time scales due to its intrinsically disordered nature. The relaxation dynamics of the amyloid-β protein and its mutants is quantitatively correlated with its experimentally measured aggregation propensity. The protective mutant has slower relaxation dynamics, whereas the causative mutants exhibit faster global dynamics compared with that of the wild type amyloid-β. The local dynamics of the amyloid- β protein or its mutants is governed by a complex interplay of the charge, hydrophobicity, and change in the molecular mass of the mutated residue.

Carbon Nanotube Network System for Reservoir Computing

Marissa Dierkes[1], Natalie O.V. Plank[1,2]
[1]Victoria University of Wellington, Wellington, New Zealand, [2]The MacDiarmid Institute, , New Zealand

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Neuromorphic networks draw inspiration from biological neural networks to implement highly efficient next-gen systems for information processing. Reservoir computing is a computational paradigm which has been shown to be favorable for processing time-dependent information and is simple to implement and easy to train [1,2]. Physical networks of highly interconnected, stochastically arranged memristive elements have been explored for reservoir computing applications due to their ability to non-linearly transform electrical input signals into high-dimensional separable outputs[3-6]. The collective behavior of these systems shows behavior similar to biological neural networks including critical dynamics (1/f noise, avalanche criticality, power-law dynamics) as well as memory properties (resistive switching) [7-9].

Here, we investigate a novel material system, based on an underlying carbon nanotube network, for its use as a physical reservoir. We demonstrate key device parameters for use in reservoir computing applications including non-linearity, resistive switching, and power-law dynamics.

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N-heterocyclic carbene as a coordinating moiety between metal nanoparticles and spin crossover compounds in nanostructured hybrid materials for neuromorphic learning

Mr Daniel Galvis[1]
[1]Lpcno, Toulouse, France

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

The neuromorphic analogy, inspired by the functioning of the nervous systems, is a promising strategy for developing more efficient and less energy-consuming hardware for computers. In such an approach, hybrid materials can be seen as an opportunity to use metal nanoparticles as neuron equivalents and molecular compounds as synapse equivalents. In this work, we studied the association between ultra-small < 3 nm platinum nanoparticles (PtNPs) and FeII triazole spin-crossover coordination polymer synthesized via self-assembly. The nanostructured hybrid materials were characterized by microscopic, magnetic, and spectroscopic techniques. The coordination of the molecular polymer was achieved via N-heterocyclic carbene moieties, which enables strong interactions with the PtNP surface. The influence of this interaction strength was studied in comparison to previous literature reports, where a thiophene functionalization was used. This work will give insight on the importance of the control of the interaction strength between metal nanoparticles and functional coordination polymers, in a neuromorphic analogy.

Evaluation of Calcium/Lithium-based Metal-Organic Frameworks for Gas Adsorption by p-DFT and Vibrational Mode Analysis

Mr Jake Gilchrist[1]
[1]University Of Otago, Dunedin, New Zealand

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Metal-organic frameworks (MOFs) based on low molecular weight metals such as lithium and calcium have been the focus of fewer studies than transition metal-based materials. Li and Ca-MOFs are proposed to possess major benefits for gas-sorption applications, including low-toxicity, high-porosity and high-stability.(1) However, these properties have not been fully characterised in the laboratory. Here we present our findings for Ca-HNCPP, a novel compound that has been synthesised at the University of Otago and designed with specific ligand binding sites to target gas sorption.

By using periodic-DFT calculations and vibrational mode analysis, we locate and quantify the binding of various atmospheric and hydrocarbon guest molecules within the pore structure of low-weight MOFs. Model vacuum and occupied unit cell geometries are optimised to allow calculation of frequency and thermochemical data to quantify important properties (binding sites and binding energy, simulated IR spectra and vibrational mode shifts). Experimentally, FTIR spectroscopy is performed on the materials in a high temperature/high pressure cell, where loading of target gases up to five atmospheres is performed.(2) Our recorded IR spectra display clear loss of solvent and residual atmospheric gases as the material undergoes vacuum activation. From subsequent gas loading experiments, host-guest interactions result in shifts in peak positions, aligned with the strength of the intermolecular interaction with the host.

By identifying the binding capability of calcium/lithium-based MOFs to CO2, C2H2 and CH4, these data can be used to improve the design of linker molecules in future iterations, to optimise gas uptake for future separation and sequestration applications.

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A soft hybrid material for self-powered and static tactile sensing

Professor Chang Soo Han[1]
[1]Korea University, Seoul, South Korea

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

In tactile sensors, self-power and static response seem like trade-offs that are never achieved simultaneously. Piezoelectric and triboelectric sensors with self-power capabilities typically respond only to dynamic stimuli, not static ones. Capacitive and piezoresistive sensors, on the other hand, provide a static response but require significant power. In this talk, we present a sensor capable of self-powering and static response using a soft hybrid material composed of ionic and piezoelectric materials. We will try to explain the novel mechanism that takes place in this device. The combined interaction of dipole-induced charge and ion migration is proposed as a plausible mechanism to understand this response. In any case, this sensor shows a slow adaptive response, just like bio-tactile sensation. In this study, soft materials such as piezoelectric gels and PVC ionic gels were used to realize the flexible device. As a result, the sensor responds statically to pressure stimuli without power consumption, which is crucial for mimicking biological tactile sensations. Furthermore, the sensor can be utilized in applications that require human tactile sensations, such as prosthetic hands, robotic hands, AR/VR, and human-machine interface devices.

Investigating the Influence of Matrix Stiffness on Chondrocyte Behaviour through Tuneable Alginate Hydrogels

Miss Maede Hasannasab[1], Associate Professor Jenny Malmström[1], Associate Professor Sue McGlashan[1], Professor Ashvin Thambyah[1], Dr Alireza Akbarinejad[1]
[1]The University of Auckland, Auckland, New Zealand

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

The mechanical properties of the extracellular matrix (ECM) play a crucial role in regulating chondrocyte behaviour, with matrix stiffness being a key factor influencing cell fate, and function. This study aims to elucidate the effects of varying matrix stiffness on chondrocytes by employing alginate-based hydrogels with tunable mechanical properties. We have achieved a range of stiffnesses by systematically altering alginate concentrations and calcium ion content, which directly impact the gel's crosslinking density. Characterisation of the hydrogels is performed at both macro and micro scales. Macro characterisation includes rheology to assess viscoelastic behaviour and compression testing for bulk mechanical properties. Micro characterization is conducted using Atomic Force Microscopy (AFM) to map surface stiffness at the nanoscale. Our research focuses on encapsulating mouse-derived chondrocyte cells within these hydrogels to explore the cellular responses to different stiffness environments. This will be evaluated through cell viability staining, imaging to observe cell morphology and attachment, and gene expression profiles associated with cartilage-specific markers. The outcomes of this study are expected to contribute to a deeper understanding of the role of matrix stiffness in cartilage biology and offer valuable information for the development of biomaterials for cartilage tissue engineering.

AI-based automatic process flow diagram generation model for interaction of academia and industry

Mr. Byeongmin Ha[1], Dr. Jou-Hyeon Ahn[1], A/Prof Soonho Hwangbo[1]
[1]Gyeongsang National University, Jinju, South Korea

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Developing a Process Flow Diagram (PFD) and a Piping and Instrumentation Diagram (P&ID) is crucial in the design of a chemical process plant. A PFD focuses on the major equipment, while a P&ID includes all the equipment, valves, piping, control structures, and more. Although P&IDs are vital for construction, engineering, and maintenance in the industry, PFDs are primarily used in academia for process development. This difference between industry and academia can be a limitation, which discourages effective interaction in knowledge transfer and collaborative projects. Therefore, P&IDs need to be converted into PFDs, but this task is time-consuming and tedious. To relieve this limitation, we propose a transformer-based AI model to generate PFDs. The AI model is designed to 1) convert text into a PFD and 2) convert a P&ID into a PFD. The purpose of text-to-PFD translation is to quickly create a sample PFD for a specific process, allowing for the development of more complex chemical plants while saving time and resources. The purpose of P&ID-to-PFD translation is to extract the main equipment from the P&ID to create a simplified PFD that can be more easily understood and analyzed. This model is expected to make communication between industry and academia easier and reduce the need for extensive human resources and time-consuming tasks. Consequently, the proposed model is anticipated to accelerate the development of chemical engineering.

Exploring the dual-doping effects of Zn and Te in the Skyrmion hosting system of (Cu1-xZnx)O(Se1-yTey)O3

Ms Branwen Hastings[1, 2], Mr Marco Vas[1, 2], M. Giansiracusa[3], C. Ulrich[4], S. Yick[1, 2], T. Söhnel[1, 2]
[1]School of Chemical Sciences, University of Auckland, , , [2]MacDiarmid Institute for Advanced Materials and Nanotechnology, [3]School of Chemistry, University of Melbourne, [4]School of Physics, University of New South Wales, Australia

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Skyrmion-hosting materials have been of increased interest in the area of spintronics. A skyrmion is a topologically protected spin-like texture and have magnetic moments that are ordered in a spiral pattern approximately 10-100 nm in size.1 Cu2OSeO3 was the first insulating helimagnet material found to host skymions.1 Due to its magnetoelectric properties, Cu2OSeO3, individual skyrmions can be controlled through applying an external electric field.2 Skyrmion hosting materials have been proposed as solutions for many current global issues, especially around energy consumption and usage, with the potential for skyrmion hosts to provide more energy-efficient memory devices with quicker storage and retrieval of information.

The aim of the current research was to investigate the effects of dual doping Cu2OSeO3 with Zn and Te, allowing for a further understanding of the formation of skyrmions. The substitution allows for the crystal structure to adjust for different ion sizes, which vary with the number of electrons or charges on the ion. Structural adjustments are made via expansion or shrinking to accommodate a difference in charge.3 Te4+ will result in the expansion of the unit cell as it is larger than Se4+. Zn2+ substitution will lower the magnetic moment, as it is non-magnetic which is different to Cu2+.

Polycrystalline of (Cu1-xZnx)2OSe1-yTeyO3 [$\Delta x = 0.025; 0 \leq x \leq 0.2$] [$\Delta y = 0.05;0 \leq y \leq 0.2$] were prepared through solid state reaction. The polycrystalline materials were analysed, with the findings of showing that the inclusion of dopant affects the optical, structural and magnetic properties of the system. Lattice expansion was observed as structural distortion occurred with the addition of dopants. There was a decrease in the band gap with increased doping. A decrease in the magnetic saturation was also found along with significant changes in the 0 field magnetisation vs temperature.

Acoustic pump-probe microfluidic device

Logan Henderson[1], Jordan Hay[1], Volker Nock[1], Linda Chen[1], Gary Turner, Joe Chen[1]
[1]University Of Canterbury, Christchurch, New Zealand

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

We describe the design and construction of a device to study the effect of ultrasonic waves in cells, protein crystals, and other biological materials. Sound waves generated by piezoelectricity is sent transversely through a microfluidic channel, acting as the pump. Optical or X-ray radiation can be sent vertically through the same channel, acting as the probe. Acoustic/optical/x-ray pump-probe experiments can thereby be enabled for time-resolved experiments to characterise materials flowing through the channel.

Development of non-toxic AgInS2 quantum dots for luminescent solar concentrators in zero-emission buildings

Mrs Sandhuli Hettiarachchi[1], Dr. Zhi Li Teh[1], Ms. Aarti Aarti[1], Associate Professor Koushik Venkatesan[1], Prof. Shujuan Huang[1]

[1]Faculty of Science and Engineering, Macquarie University, Sydney, Australia

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Luminescent solar concentrators (LSC) are crucial in building integrated photovoltaics (BIPV), harnessing solar energy through windows to contribute to net-zero-energy buildings[1]. Semiconductor nanoparticles called quantum dots (QD), are promising candidates for LSCs[2] owing to their high light-emitting efficiency. Since many efficient QDs contain toxic heavy metals, developing non-toxic alternatives is imperative. Ternary QDs with I-III-VI elements show significant potential in this context[3]. This study aimed to synthesize non-toxic, high-light emission $AgInS_2$ QDs for LSCs. Hot-injection method was used with varying sulfur injection temperatures (120°C, 140°C, 160°C, 180°C, and 200°C). Transmission electron microscopy (TEM) images showed increased QD size (3.03-6.19 nm) with increased injection temperature. The band gap decreased (2.79-1.98 eV) due to quantum confinement[4] and photoluminescence (PL) emission peak red-shifted from 585 to 735 nm. PL quantum yield (PLQY) was maximum (54.45%) in QD synthesized at 180°C injection temperature. To further increase the PLQY, ZnS shell was synthesized forming type I core/shell QDs. The PLQY increased to 63.67% due to surface passivation by ZnS shell. PL peak blue-shifted (from 660 nm to 626 nm) due to core-size shrinkage with cation-exchange during shelling. In conclusion, AgInS2 QDs with tuneable emission were synthesized, and enhanced PLQY was observed upon shelling, forming AgInS2/ZnS QDs. These luminescent non-toxic QDs will be used in LSC for optimum sunlight harvesting.

Keywords: Non-toxic, quantum dots, hot injection method, photoluminescence, quantum yield.

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Exploring Structural Variability in Tri-HBC Compounds: Implications for π-Stacked Porous Solid Design

Miss Panchami Hirave, Prof. Nigel Lucas
[1]MacDiarmid Institute of Advanced Material Science and Nanotechnology and Department of Chemistry, University of Otago, Dunedin, New Zealand, 9016.

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Over the past two decades, the development of porous materials has seen remarkable progress, particularly with the advent of metal-organic frameworks (MOFs) and covalent organic frameworks (COFs). These materials, formed through strong coordination or covalent bonds, offer customizable thermal and chemical stabilities, pore sizes, shapes, and functionalities.[1] In contrast, supramolecular organic frameworks (SOFs) assemble through non-covalent interactions such as hydrogen bonding and π stacking.[2] While hydrogen bonding has been extensively utilized in SOFs, the exploration of porous organic solids primarily driven by π-stacking interactions remains limited.[3] Hexabenzocoronene (HBC) is a symmetrical polycyclic aromatic hydrocarbon (PAH) composed of 42 carbon atoms. It exhibits properties of a donating group due to its dense π electron system and possesses a large bandgap.[4] Compared to other PAHs, HBCs feature a wider bandgap attributed to a stable resonance structure where π electrons are delocalized across separated rings, adhering to Clar's aromatic sextet rule.[5] HBCs have garnered significant interest due to their unique electronic properties and their tendency to self-assemble into discotic liquid crystalline phases.[6] The self-organization capability of HBCs is highly influenced by the nature of the substituents attached to the periphery of their molecular structure. Systematic structural modifications can be utilized to evaluate the stability of the crystalline π-stacking motif and ascertain whether the three-dimensional crystalline integrity can be improved through stronger interlayer interactions. The microstructure of these carbon-rich compounds can be analyzed using X-ray crystallography and Raman spectroscopy on both bulk and solution samples.

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Harnessing Solvent-Induced Browning Chemistry of Amino Acids for Nanoparticle Synthesis and Drug Delivery Applications

Dr Teh-Min Hu
[1]Department of Pharmacy, National Yang Ming Chiao Tung University, Taipei, Taiwan

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Amino acids, with their natural abundance and well-characterized properties, present significant potential as biomaterials. In this study, we introduce a novel method for synthesizing nanoparticles using amino acids as starting materials. The amino acids undergo an extensive browning reaction in a solvent mixture of dimethyl sulfoxide (DMSO) and acetone at room temperature. This unique browning process diverges from the traditional Maillard reaction, as it occurs in non-aqueous, aprotic solvents without the need for intense heating or the presence of reducing sugars. Our previous research demonstrated that this reaction involves amino acids acting as organocatalysts, facilitating the self-aldol condensation of acetone in DMSO. This organocatalytic process transforms amino acids into a complex array of compounds, characterized by an intense brown color. The resulting browned amino acid derivatives exhibit significant hydrophobicity, enabling the formation of nanoparticles in water via nanoprecipitation. These spherical nanoparticles, with diameters ranging from 100 to 200 nm, display pH-switchable charge-reversible properties and antioxidative capabilities. In this presentation, we will share new data that further elucidates the characteristics of this innovative nanoplatform, particularly its potential applications in drug delivery systems.

Promoting Bone Regeneration with ECM-Functionalized Titanium Surfaces Mimicking Biomimetic Elastic Proteins

Dr Jun-hyeog Jang[1]
[1]Inha University School of Medicine, Incheon, South Korea

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Titanium, renowned for its exceptional mechanical and chemical properties, lacks sufficient bioactivity. To enhance cellular response and osseointegration, the titanium surface was functionalized to replicate an ECM-like microenvironment, crucial for stem cell behavior modulation. However, native ECM components like fibronectin and elastin are impractical due to cost and immunogenicity. Addressing these challenges, a recombinant chimeric FN-ELP was developed and applied, resulting in sustained bioactivity and enhanced osteogenic differentiation of hMSCs, promising improved bone regeneration.

Contrast enhanced NIR-II photoacoustic imaging with barium sulfate and pigment admixture

A/Prof Mansik Jeon[1], Mr Yoonseok Kim[1], Prof Jin-Seok BAE[2], Prof Mansik Jeon[1], Prof Jeehyun Kim[1]
[1]Department of Electronic and Electrical Engineering, Kyungpook National University, Daegu, South Korea,
[2]Department of Textile System Engineering, Kyungpook National University, Daegu, South Korea

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

In biomedical imaging, a substrate that alters image contrast in a meaningful way that helps to distinguish between normal and abnormal conditions is known as a contrast agent. A range of biomedical applications employs multimodal imaging contrast agents, which enhance the contrast of structures or fluids in biomedical imaging. Due to the capabilities of enabling deep penetration imaging with minimal tissue scattering in the 1000 to 1700 nm wavelength range, optical contrast agents that absorb in the NIR-II have shown potential in photoacoustic imaging (PAI). In this study, to facilitate preclinical imaging using PAI modality, a dual-modality contrast agent was developed comprising an admixture of barium sulfate with dyes that absorb light in NIR-II. 1064 nm Q-switched Nd:YAG microchip laser-based PAI was used. Barium sulfate and barium sulfate with dye (NIR-II dye) were subjected to PAI for evaluating the PA intensity signal properties of the micro-particle and micro-particle with dye. In addition, the activation process of the micro-particle was monitored for five minutes. No PA signal was detected when the particle was imaged alone, but a strong PA signal was detected when the particle was imaged with dye. Based on the analysis data, the average PA signal of the particle with dye is continuously increased compared to the particle alone. Moreover, the region of generating PA signal was broadened while time passed because of the aggregation. We expected that this dye has a high utility in different animal models for functional imaging purposes.

Computational Study of Carbonation Reaction for Carbon Capture and Storage in Concrete

Professor Sohdam Jeong[1]
[1]Dong-eui university, Busan, South Korea

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Concrete, as a primary constituent of architectural structures, generally plays a crucial role in their durability and stability. The carbonation reaction, one of its main reactions, refers to the dissolution of hydrates releasing calcium ions into solution, which react with dissolved carbonates to produce $CaCO_3$, thereby influencing the material's long-term performance. However, when properly directed and controlled, carbonation can be beneficial for applications such as carbon capture and storage (CCS) or self-healing. Therefore, we investigate whether reinforced concrete allows CCS, thereby controlling the carbonation reaction in concrete. Because of a lack of reliable predictive models linking the chemistry of carbonation at the molecular scale to microstructure development and macroscopic properties, here we construct the theoretical modeling of the carbonation reaction based on density functional theory to elucidate the underlying molecular mechanisms. We calculate the transition states and reaction paths of the main reactions under different environmental conditions, with thermodynamic and structural properties. We hope that this research will facilitate the precise control of carbonation reactions in concrete, enhance the durability of architectural structures, and finally make contributions to CCS, or self-healing concrete applications.

Unravel the Sugarcoating; Surface patterning with unprotected sugars towards mimicking the glycocalyx

Mr Jude Kalan[1]
[1]University Of Canterbury, Christchurch, New Zealand

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Sugars play critical roles in cellular communication and identification[1]. The layer of cell surface oligosaccharides present on the cell membrane is referred to as the glycocalyx. The oligosaccharide, the biological structure they are attached to, as well as their spatial relationship to other glycoconjugates, all impact binding affinities and selectivity between cells and exogenous biomolecules. This results in the glycocalyx being a complex network that is crucial for cellular communication that needs to be fully understood.

Current studies on the glycocalyx are typically done in vivo, but this approach is difficult and a reliance on internal glycosylation machinery, hence the desire to create a glycocalyx model on solid substrates. Building on existing microfabrication technology, this project aims to develop methodology to create bespoke glycocalyx models on solid surfaces. This will be done by patterning the surface with unprotected sugars. Using Barner-Kowollik's[2] photoactivated Diels-Alder reaction, glycans can be covalently linked to a surface with spatial control. This can be repeated with other glycans positioned within nanometres of each other to create a more realistic model of the glycocalyx.

A surface that has been functionalized with this aryl aldehyde compound can be protected with photomasks to control which sites are exposed to light. This would dictate where the ligation of the sugar occurs. Repeating this with other photomasks and other sugars will start to build up a complex model of the glycocalyx. Work to date includes development of the synthetic precursors, and functionalization of the surface in anticipation of covalently bonding sugars to it.

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Anti-Fouling Properties of Phosphonium Ionic Liquid Coatings in the Marine Environment

Mr Sajith Kaniyadan Baiju[1,2,3], Mr Brent James Martin[4], Mrs Rayleen Fredericks[1,2,3], Mr Harikrishnan Raghavan[1,3], Dr Karnika De Silva[5], Dr Matthew Greig Cowan[1,2,3]
[1]Department of Chemical and Process Engineering, University of Canterbury, Private Bage 4800, Christchurch 8140, New Zealand, [2] New Zealand Product Accelerator, University of Canterbury, Private Bag 4800, Christchurch 8140, New Zealand, [3] MacDiarmid Institute for Advanced Materials and Nanotechnology, University of Canterbury, Private Bag 4800, Christchurch 8140, New Zealand, [4] Defense Technology Agency (DTA), Private Bag 32901, Auckland 0744, New Zealand, [5] NZ Product Accelerator, Faculty of Engineering, University of Auckland, Auckland 1010, New Zealand

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Biofouling, the unwanted accumulation of marine life on submerged structures, continues to pose a significant economic burden to many marine industries.[1] This research explores the potential of phosphonium ion gels as a novel anti-fouling solution. Specifically, biocide potential was correlated with alkyl chain length, hydrophobicity, and copper content of the ion gels.

A series of ion-gels were created using varying concentrations of phosphonium monomers with the biocidal anion [AOT]-. The monomers ([P444VB] [AOT] and [P888VB] [AOT] (50-90 wt.%) and free ionic liquids ([P4448] [AOT], [P88814] [AOT]); 10 to 50 wt.%), were used to prepare the gels through photopolymerization. These gels were tested in a seachest simulator in New Zealand coastal waters, protected from light and tides, over the summer and autumn months.[2]

The results showed that more water-repellent gels, achieved through reduced free ionic liquid and longer alkyl chain components, performed better at preventing biofouling. Surprisingly, adding copper biocide hindered performance by making the surface more hydrophilic. These results therefore suggest that hydrophobicity plays a major role in the long-term anti-fouling of marine surfaces. Additionally, no direct correlation was found between antimicrobial activity and anti-fouling efficacy.[2]

In conclusion, this research underscores the potential of phosphonium ion gels as a promising avenue for combining anti-fouling and foul-release properties, these gels could offer a new way to tackle this persistent marine problem.[2]

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Ion beam tuning of optical properties of halide perovskites

Dr John Kennedy[1,2], Dr Holger Fiedler, Dr Jake Hardy
[1]National Isotope Centre, GNS Science, Lower Hutt, New Zealand, [2]The MacDiarmid Institute for Advanced Materials and Nanotechnology, New Zealand

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Ion implantation is a highly precise method for modifying the properties of inorganic semiconductors. Low-energy ion beam modification enables the precise formation of point defects near the surface, which are typically considered detrimental to light-harvesting applications. However, halide perovskites have been shown to exhibit significant resistance to radiation damage, with those used in solar applications demonstrating a surprisingly high defect density.

In this study, we demonstrate the tunability of photoluminescence lifetime and photoluminescence quantum yield (PLQY) through ion beam modification. At low fluences of 10^{13} at.cm^{-2} at 20 keV, an enhanced PL lifetime emerges for large ions, while small ions can boost the PLQY of halide perovskites. We discuss the structural origins of this universal effect on halide perovskites, based on ion beam-substrate interactions (Monte Carlo simulations), complemented by x-ray diffraction (XRD), UV-Vis, and atomic force microscopy (AFM) investigations.

This research facilitates the exploration of subtle variations within the perovskite structure and presents a pathway to address the critical manufacturability and stability challenges plaguing perovskite devices.

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Composite polymer electrolyte with surface-functionalized silica mesoball fillers

Dr Jae Hyun Kim[1]
[1]Dgist, Daegu, South Korea

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Mesoporous silica (SMB) has dual benefits, namely, it is cost-effective, offers an extensive surface area (≈905 m 2 g−1), and has been used as a filler. Surface modification of the fillers improves the dispersity of Li salt in the solvent, which improves the compatibility of the solid state electrolytes with the Li metal. The modified silica micro-ball (MSMB)material, which has a high level of porosity, has dual functionalities: It acts as a plasticizer that expands the amorphous polymer regions, thereby enabling Li-ion transportation and provides ample interaction sites by maintaining good dispersion in the polymer matrix. Therefore, with the appropriate surface modification of the SMB, the effectiveness of the MSMB-based CPE (MSMB-CPE) is exploited. The MSMB-CPE of ionic conductivity of 1.16 × 10−2 S cm−1 @60 °C and a venerable Li-ion transference number of 0.81 were obtained

Cellulose-Based Dispersion of Single-Walled Carbon Nanotubes for Solution Processing Applications

Mr Joonyoup Kim[1,2], Mr Minkyun Kang[1,2], Prof Yongtaek Hong[1,2]
[1]Department of Electrical and Computer Engineering, Seoul National University, Seoul, South Korea, [2]Inter-University Semiconductor Research Center (ISRC), Seoul National University, Seoul, South Korea

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Carbon nanotubes (CNTs) are suitable candidates in numerous applications including nanocomposites, electronics, and optical devices due to their exceptional properties[1]. However, their aggregation in aqueous solutions, caused by hydrophobic interactions and strong van der Waals forces, makes the process difficult to implement[2]. Conventional dispersion methods, such as chemical functionalization and surfactant addition, either alter the nanotubes' electronic properties or weaken their interaction with polymers[3, 4].

In this study, we explore the use of cellulose as an alternative dispersant for single-walled carbon nanotubes (SWCNTs). Cellulose, the most abundant organic polymer on Earth and derived from renewable sources, provides a unique advantage by facilitating hydrophobic interactions and long-range electrostatic repulsion[5], which enable the effective dispersion of SWCNTs in water. We compared cellulose’s dispersion performance with that of the conventional surfactant sodium dodecyl sulfate (SDS). The results demonstrate that cellulose achieves excellent dispersion of SWCNTs at lower concentrations, while maintaining their inherent graphitization purity and facilitating the creation of stable, highly conductive dispersions. Furthermore, the cellulose/SWCNT dispersions were effectively employed in solution processes such as spray-coating and inkjet printing. Spray-coating produced ultrathin films with tunable conductivity and high transmittance, while inkjet printing facilitated stable droplet formation and uniform film creation by optimizing printability through control of cellulose concentration. The prepared cellulose/SWCNT dispersions not only improve the dispersion of SWCNTs but also facilitate the development of advanced materials for various applications, demonstrating their potential as an eco-friendly solution for processing.

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Asymmetric gradient orbital interaction of hetero-metal active sites for promoting photocatalytic C−C coupling processes

Professor Taekyu Kim[1]
[1]Korea Advanced Institute of Science and Technology (KAIST), Daejeon, South Korea

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Diatomic-site catalysts (DACs) garner tremendous attention for selective CO2 photoreduction, especially in the thermodynamical and kinetical mechanism of CO2 to C2+ products. Here we present the engineering of a novel Zn-porphyrin/RuCu complex DAC (ZnPor-RuCuDAC). The heteronuclear ZnPor-RuCuDAC exhibits the best acetate selectivity (95.1%), while the homoatomic counter-parts (ZnPor-Ru2DAC and ZnPor-Cu2DAC) present the best CO selectivity. The in-depth analyses confirm that due to the strong gradient orbital coupling of Ru4d–Cu3d resonance, two formed *CO intermediates of Ru–Cu heteroatom show a significantly weaker electro-static repulsion for an asymmetric charge distribution, which result from a side-to-side absorption and narrow dihedral angle distortion. The strongly overlapped Ru/Cu-d and CO molecular orbitals split into bonding and antibonding orbitals easily, resulting in decreasing energy splitting levels of C1 intermediates. These results collectively augment the collision probability of the two *CO intermediates on heteronuclear DACs.

Effect of Structural Characteristics and Molecular Weights of Biscarbazole-based HTMs on Photovoltaic Performance of Solid-State DSSCs

Professor Younghwan Kwon[1]
[1]Daegu University, Gyeongsan, South Korea

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Dye-sensitized solar cells (DSSCs) have limited their long-term performance due to the potential problems of leakage and liquid volatilization of liquid electrolytes. Solving these problems caused by liquid electrolytes requires replacing the liquid electrolytes in DSSCs with a solid-state hole-transporting material (ssHTM). Many carbazole derivatives have been applied as HTMs on organic electronics because of their excellent hole-transporting capabilities and chemical stability. Carbazole moiety represents a good electron-donating nature due to the nitrogen atoms' presence, which accounts for its derivatives' superior hole mobilities. In this study, solution-processable conjugated poly[N-(2-ethylhexyl)-3,6-carbazole-alt-aniline] copolymers containing alternating carbazole and triarylamine moieties are synthesized in a good yield by Pd-catalyzed polycondensation, because both of carbazole and triarylamine groups have been known to have hole-transporting performance. poly[N-(2-ethylhexyl)-3,6-carbazole-alt-aniline] copolymers with different molecular weights are applied in combination with additives to produce solid-state DSSCs. The PCE of the ssDSSC with higher molecular weight HTM was increased due to higher hole mobility and electrical conductivity of HTM. This result indicates that a higher-molecular-weight polymeric HTM is a better choice to obtain superior photovoltaic performance in ssDSSCs.

Keywords: Dye-sensitized solar cell, Redox mediator, Organic-solvent free, Co complex, Ionic liquid

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Monovalent ion-selective membranes with enhanced interlayer adhesion

Ms. Ji-Hyeon Lee[1], Ms. Hyeong-Bee Song[1], Professor Moon-Sung Kang[1]
[1]Sangmyung University, Cheonan-si, South Korea

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Ion-exchange membranes (IEMs) that selectively transport cations or anions are extensively used in water treatment and electrochemical energy conversion processes. Many electrochemical membrane processes often require selective permeation properties for specific ions in addition to the basic separation properties of IEMs [1]. To improve the selective permeation properties of IEMs for specific ions, there are methods such as chemically modifying the surface of the base membrane or coating a thin layer with high permselectivity [2]. However, the surface-modified layer can increase the overall electrical resistance and can easily be separated from the base membrane. Therefore, in this study, we aimed to develop an IEM that improves the interfacial stability of the base membrane and the surface-modified layer, does not increase the electrical resistance of the membrane, and consequently significantly improves the permselectivity for specific ions. To this end, polydopamine (PDA), which has excellent interfacial adhesion, was selected as the basic material for surface modification [3]. In addition, various hydrophilic polymers containing carboxyl, alcohol, and amine groups were combined with PDA to appropriately control the hydrophilicity and electrostatic repulsion of the membrane surface. The prepared composite membrane was systematically analyzed through various electrochemical methods, and its performance was evaluated by applying it to water-splitting electrodialysis for recovering acids and bases from salts. The results showed that the fabricated composite membranes exhibited superior levels of monovalent ion selectivity and electrochemical properties compared to commercial membranes. This work was supported by NRF grants funded by the Government of Korea (MEST) (NRF-2022M3C1A3081178 and NRF-2022M3H4A4097521).

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A New Pixelation Method Using Ag Thin Film within a Tandem Structure for High-Resolution Full-Color Quantum Dot Light-Emitting Diodes

Mr Kwangkeun Lee[1], Mr Yeoungmin Moon[1], Mr Taewoong Yoo[1], Professor Jeonghun Kwak[1]
[1]Seoul National University, Seoul, South Korea

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Quantum dot (QD) light-emitting diodes (QLEDs) are considered a promising next-generation display technology1. To realize full-color QLEDs, the patterning of red, green, and blue QD EMLs, which is essential for pixelation, is mainly facilitated by solution-based processes such as inkjet printing, transfer printing, and photolithography.2-4 However, despite extensive research on QD EML patterning using solution-based processes, there are still limitations in achieving high-resolution QLEDs.2 Herein, we present a new method for QLEDs

pixelization without QD EML patterning by using a 25 nm thick Ag thin film in a stacked tandem structure composed of ITO/ZnMgO/Red QD/TCTA/MoO3/Ag/ZnMgO/Green QD/TCTA/MoO3/Al. The Ag layer, which is deposited by a vacuum deposition process that is advantageous for forming more precise patterns than solution process patterning, functions not only as an electrode but also as a pixelation layer.

As a result of this strategy, we demonstrated pixelated InP-based QLEDs with red and green pixels driven by applying signals to ITO (cathode) and Ag (anode) for the red pixel and Ag (cathode) and Al (anode) for the green pixel, respectively. The red pixel exhibits a maximum external quantum efficiency (EQEmax) of 4.8% and a maximum luminance (Lmax) of 31,030 cd/m2, and the green pixel exhibits an EQEmax of 2.8% and a Lmax of 5,840 cd/m2. We believe that our results provide insight into an efficient and simple method for achieving high-resolution full-color QLEDs.

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Precursor crystalline structure from organic pigment red 122 for polysulfide confinement and conversion in lithium–sulfur batteries

Professor Seung Geol Lee[1], Mr Woo Sub Heo[2]
[1]Ulsan National Institute of Science and Technology (UNIST), Ulsan, South Korea, [2]Pusan National University, Busan, South Korea

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Lithium-sulfur batteries (LSBs) hold significant promise for high energy storage applications; however, they encounter challenges such as limited sulfur utilization and poor cycling stability, primarily due to the lithium polysulfides (LiPSs) shuttle effect. We prepared nitrogen/oxygen-doped activated carbon hosts for LSBs using an eco-friendly one-step activation process. Unlike other precursors, pigment red 122 (PR) offers high activation yield and large surface area due to its good crystallinity and strong molecular interactions. Functionalization with nitrogen and oxygen was facilitated by PR's amine and hydroxyl groups. By varying the PR weight ratio (APR_X, X=1:1, 1:3, 1:5), we achieved different surface areas and pore sizes. Notably, APR_1:5 delivered 804 mAh g^{-1} after 200 cycles with over 99% coulombic efficiency at a current density of 0.2 C, outperforming other APR electrodes. This superior performance is attributed to its rational pore sizes and larger surface area, which effectively trap and suppress LiPSs and mitigate the shuttle effect. Our method highlights the synergistic effect of precursor crystallinity and molecular structure, paving the way for efficient carbon-based sulfur hosts in high-performance LSBs.

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Dual modification of high-voltage LiFe0.4Mn0.6PO4 cathode for accelerated low-temperature kinetics

Professor Youngil Lee[1]
[1]University Of Ulsan, Ulsan, South Korea

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Olivine cathode is considered a promising material due to its moderate theoretical capacity, low cost, and environmental friendliness. The main drawbacks of olivine cathode include poor electrical conductivity and sluggish Li-ion diffusion during discharge due to its restricted one-dimensional ion transport, which significantly hinders the (de)lithiation process, resulting in energy and capacity loss. These drawbacks become more severe at low temperatures. Focusing on the multicomponent olivine LiFe0.4Mn0.6PO4 (LFMP), we found that its performance at low temperatures was strongly affected by the Fe-Mn redox exchange. The redox exchange induced polarization and terminated the cell performance. By providing a Li1.3Al0.3Ti1.7(PO4)3 (LATP) solid electrolyte, the composite LFMP_LATP coated with carbon and LATP (LFMP_LATP@C_LATP) mitigated the inferior Li-ion diffusion to remarkably improve the capacity delivery and cycling stability at low temperatures.

Spectroscopic and Computational Investigation of the Efficient Formation of Glycine on Olivine and Ice Surfaces in Interstellar Environments.

Mr Jacob Lewis[1], Assoc. Prof. Anna Garden[1], Dr. Courtney Ennis[1]
[1]University Of Otago, Dunedin, New Zealand

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

The identification of amino acids in space has so far been tentative at best, with no confirmed detections outside of Earth. Detecting one such as glycine, is like finding a 10-atom needle in the largest and darkest haystack, thus narrowing down the search is key. Interstellar space cycles through stages of evolution, from cold sparse molecular clouds to hot cores of gas and planetary systems, each with different chemistry that may produce amino acids. Determining which of these environments may produce significant amounts of glycine provides insight to where interstellar amino acids could be detected.

The most abundant surfaces in such environments are silicate mineral grains, such as olivine, and water ice. Many of these regions are rich in small molecules such as methylamine, which is thought to be formed and potentially react on surfaces to form larger organics. Glycine formation from methylamine (CH3NH2) and formic acid (HCOOH), and their dehydrogenated counterparts, will be investigated as these are the simplest bimolecular precursors of the simplest amino acid.

The reactions between precursors on the surfaces will be investigated using a combination of theoretical and experimental methods. The potential reaction mechanisms will be explored, and reaction thermodynamics and kinetics calculated, using DFT. While experimentally, a vacuum chamber will be used to reproduce the conditions within both the cold and hot environments. Irradiating the interstellar surfaces and precursors with UV light, and monitoring with IR and MS. From this information, the environment and reactions that could produce interstellar glycine may be better understood.

Slip flow of concentrated emulsions in microchannels: Effects of surface wettability

Mr Ssu-Kai Li
[1]National Taiwan University, Taipei, Taiwan

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Concentrated emulsions can be applied in droplet microfluidics for cell culture, enzyme reaction kinetics, etc. They exhibit complex flow characteristics in microchannels, with wall slippage often being prominent. In this work, the slip flow of monodisperse concentrated emulsions, affected by the surface wettability of channel walls, is investigated using dissipative particle dynamics. The effect of surface wettability, defined by the intrinsic contact angle (CA), on wall slippage, measured by the slip velocity, is systematically examined under identical external force. Two scenarios modifying surface wettability are considered: (i) changing wall-continuous phase affinity and (ii) changing wall-dispersed phase affinity. It is found that for various wettabilities, the flow behavior varies significantly near the wall, while essentially remaining the same away from the wall. This result can be attributed to the microstructure near the wall, which generally consists of crowded, adhered droplets rather than forming a lubricated layer. In the adsorbed layer, the apparent CA of adhered droplets differs from the intrinsic CA, and their local volume fraction differs from the bulk volume fraction. Even the same intrinsic CA, resulting from various combinations of wall-liquid affinities, may yield different microstructures and, consequently, different slip velocities. Finally, a simple model based on the sum of both wall-water and wall-oil contributions is proposed to successfully depict the simulation results.

Fascinating and special Circular Dichroism of Helical Assemblies of silver nanowiers

Mr Zheng Fong Li[1], Mr Kun Jie Zeng, Mr Yu Ying Chang, Professor Hua Shu Hsu
[1]National Pingtung University, Pingtung, Taiwan

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Chirality is a phenomenon observed at various length scales in nature, and chiral metasurfaces have garnered significant attention due to their unique optical properties and potential applications. We successfully fabricated optically chiral nanowire structures by oblique angle deposition of silver nanowire suspensions onto a quartz substrate mounted on a rotating stage, with precise control over their arrangement using simple macroscopic tools. These multilayer helical assemblies exhibited remarkable chiroptical properties, particularly strong circular dichroism (CD) in the ultraviolet region. In CD spectroscopy, we observed significant peaks at 385 nm and 343 nm. However, CD mapping at 343 nm revealed that different areas of the same sample exhibited opposite CD signals. Interestingly, after rotating the sample, the signals remained unchanged, similar to the effects of linear polarization. This unusual distribution of CD may be influenced by linear dichroism (LD), indicating substantial potential for further exploration in optical research. Our study presents a straightforward and feasible method for fabricating large-area chiral structures, with the potential to extend to more complex designs that can be finely tuned using simple design principles.

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Anomalous Magnetization Hysteresis Behavior of Thulium Iron Garnet (TmIG) under Magnetic Circular Dichroism (MCD)

Mr Wei Hsiang Liao[1], Mr Po Chun Lien[1], Ms Yu Siou Jheng[1], Mr Yu Ying Chang[1], Prof Hua Shu Hsu[1]
[1]National Pingtung University, Pingtung, Taiwan

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Iron Garnet is a type of ferrimagnetic material, characterized by ferrimagnetic coupling between tetrahedral and octahedral iron ions. Thulium Iron Garnet (TmIG), due to its perpendicular magnetic anisotropy, finds widespread applications in magneto-optical materials. In our study, we fabricated TmIG thin films and employed Magnetic Circular Dichroism (MCD) spectroscopy for analysis. The results revealed that the magnetic moments of tetrahedral and octahedral iron ions competed at different energies, leading to anomalous MCD hysteresis loops. These anomalies were observed specifically within certain spectral energy ranges, particularly near the characteristic spectral peaks of TmIG. Further investigation indicated that this phenomenon is associated with defects near the substrate in the thin film. These defects likely induce local magnetic inhomogeneities, affecting the ferrimagnetic coupling between tetrahedral and octahedral iron ions, thereby introducing additional hysteresis effects during magnetic field variation. Notably, these anomalous MCD results are not prominent in conventional magnetic measurements, as such tests often fail to capture these subtle spectral-dependent features. This finding provides critical insights into the magnetic characteristics of TmIG and aids in optimizing its performance for magneto-optical applications.

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Crystallization and Young’s Modulus of Nanofilm of Physical Elastomer Immersed in Nonsolvent: Effect of Film Thickness

Mr Chih-Jung Lin[1]
[1]National Taiwan University, Taipei, Taiwan

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Nanofilms exhibit distinct behaviors compared to bulk materials, particularly concerning the effects of film thickness on melting temperature and Young’s modulus, which are not yet fully understood. In this work, dissipative particle dynamics simulations are employed to investigate the crystallization and stiffness of nanofilms immersed in a non-solvent bath. The solid state of the nanofilm, as confirmed by consistent melting temperatures determined from the polymer's radius of gyration, heat capacity, and crystallinity, indicates that thinner nanofilms have higher melting temperatures. Through uniaxial extension, the stress-strain curve of the nanofilm is obtained, and Young’s modulus generally increases toward a plateau with decreasing film thickness. Under strain, the decrease in crystallinity correlates with increased internal energy and positive entropy change, in contrast to typical rubber elasticity where entropy decreases upon stretching. It is found that local crystallinity near the interface is significantly higher than in the central region. Both regions show an increase in crystallinity as thickness diminishes, due to the surrounding non-solvent environment enhancing polymer alignment and crystallization. As the film thickness decreases to the nanoscale, the influence of the interfacial region becomes more pronounced, thereby increasing the film’s stiffness.

Lipid nanoparticles efficiently deliver DNA vaccine to robustly induce antigen-specific immune responses

Dr Shih-jen Liu[1], Dr Hung-Chun Liao[1], Dr Chung-Hsiang Yang[1], Dr Ming-Hsi Huang[1]
[1]National Health Research Institutes, Zhunan Town, Taiwan

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DNA vaccines for infectious diseases and cancer have been explored for years. To date, only one DNA vaccine (ZyCoV-D) has been authorized for emergency use in India. DNA vaccines are inexpensive and long-term thermostable, however, limited by the low efficiency of intracellular delivery. The recent success of mRNA/lipid nanoparticle (LNP) technology in the COVID-19 pandemic has opened a new application for nucleic acid-based vaccines. Here, we report that plasmids encoding a trimeric spike protein or HPV 16 E6E7 oncogene with LNP could generate robust immune responses. Both vaccines can induce humoral and cellular immunity against SARS-Co-V2 infection or HPV-associated cancer growth in animals. Interestingly, we found that DNA/LNP can induce higher antibody titers than naked DNA or DNA delivered via electroporation. Compared to mRNA/LNP, DNA/LNP immunization induced a comparable level of neutralizing antibody titers and significant Th1-biased immunity in mice. Importantly, DNA/LNP immunization exhibits enhanced anti-tumor immunity protects from tumor challenge. The study indicates that DNA/LNP as a promising platform could be a next-generation vaccine technology.

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Comparison of CO2 photocatalytic reduction efficiency using BiAX (A=O, S, Se, Te; X=Cl, Br, I)/g-C3N4 as catalysts

PhD Yu Yun Lin[1], master Fu Yu Liu[1], Chin Hsuan Tseng[1], Professor Shiuh Tsuen Huang[1], Hong Han Huang[1], Dr YuYun Lin[1]
[1]National Taichung University of Education, Taichung, Taiwan

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

BiAX (A=O, S, Se, Te; X=Cl, Br, I)/g-C3N4 photocatalyst was successfully synthesized using hydrothermal or solvothermal methods [1,2]. The main purpose of this research is to promote the conversion of carbon dioxide into sustainable hydrocarbons (solar fuels), providing attractive solutions to environmental problems and energy crises. These photocatalysts show significant efficiency in converting CO2 to CH4, with the photocatalytic conversion rates of BiSeCl (BiSCl, BiTeCl)/g-C3N4 being 1.92 (0.16, 0.5) µmolg-1h-1, respectively. The optimized BiAX photocatalyst exhibits high selectivity in gradually converting CO2 to CH4 without detecting other oxygen-containing compounds, ultimately producing more high-value hydrocarbons (C2+). In addition, due to their ability to reduce carbon dioxide, these photocatalysts are expected to be one of the material candidates for mitigating environmental pollution.

Enhancing Advanced Material Reliability through Deep Learning: A Conceptual Framework

Professor Jung-Hua Lo[1]
[1]Fo-Guang University, Yilan, Taiwan

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

In recent years, the integration of deep learning techniques into the field of advanced materials has shown significant promise in enhancing the reliability of material properties and performance. This study explores the theoretical framework and potential applications of deep learning algorithms to predict and improve the reliability of advanced materials. By proposing a methodology that leverages large datasets and sophisticated neural network models, we aim to develop a predictive framework that can, in future work, accurately forecast the behavior and lifespan of materials under various conditions. Our approach involves conceptualizing how deep learning models could be trained on experimental data to identify patterns and correlations that traditional methods might overlook. Additionally, we draw parallels between material reliability and software reliability, suggesting that techniques used to enhance the robustness of software systems can be adapted to predict material failures. This conceptual study not only highlights the potential precision of reliability predictions but also provides insights into the underlying mechanisms that might govern material failure and degradation. Furthermore, the proposed integration of deep learning into reliability assessments could allow for real-time monitoring and adaptive control, thereby reducing the risk of unexpected failures in critical applications. Our discussion demonstrates that, despite the current lack of available datasets, deep learning offers a powerful prospective tool for advancing the field of materials science.

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Validation of Gelatine Layering Method for Ultrasound Powering and Communication

Mr Kaleb McGillivray-Seaton[1], Associate Professor Deborah Munro[1]
[1]University Of Canterbury, Christchurch, New Zealand

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Sensors are increasingly used to monitor bodily functions, collecting real-time data with minimal discomfort. Ultrasound, a wireless method requiring a propagation medium like human tissue, is utilised as a communication link [1]. Human tissue is comprised from layers of skin, fat, and muscle that vary in thickness and acoustic properties between individuals [2]. Device testing requires stable, repeatable setups, and water is thus commonly used due to its accessibility and homogeneity, avoiding issues like reflections and refractions from layer changes [3]. However, gelatine presents a viable tissue alternative, capable of being both homogeneous and heterogeneous with stable properties that may more closely represent human tissue. By creating gelatine slabs with varying properties and layering them, a human tissue substitute can be formed. This research aimed to validate a protocol for stacking gelatine slabs to create such a substitute.

The study employed Humimic Medical Gelatine #0, simulating fat, moulded into 75x75 mm slabs with thicknesses of 10, 20, and 50 mm. A 1MHz sound wave was propagated between transmitting “external” and receiving "implant" transducers, recording the voltage across them when different coupling agents were used. The coupling agents tested included water, acoustic gel, and no agent. Results indicated the necessity of a coupling agent at the gelatine-transducer boundary, with water showing less variation than acoustic gel. Between gelatine layers, using no coupling agent and a “rolling” technique for slab placement resulted in the least variation. These combined methods yielded a layered human tissue substitute that was comparable to using water.

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Sustainable Aerogels: Harnessing Canola Seed Meal Proteins

Dr Honey Gupta[1,2], Dr Steven McNeil[1], Mr Steve Ranford[1], Dr Mark Staiger[2,3]
[1]Bioproduct and Fibre Technology Group, AgResearch, Christchurch, New Zealand, [2]Department of Mechanical Engineering, University of Canterbury, Christchurch, New Zealand, [3]Biomolecular Interaction Centre, University of Canterbury, Christchurch, New Zealand

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Aerogels show promise in diverse applications due to their high specific surface areas, low density, and high strength-to-weight ratio [1-3]. Bio-based materials offer a sustainable alternative to inorganic and carbonaceous materials for the preparation of functional aerogels. The greater biocompatibility and biodegradability of bio-based aerogels opens new opportunities for applications in food, cosmetics, and the controlled release of bioactive compounds [4].

This study explored the formation of bio-aerogels from proteins extracted from canola seed meal via an aqueous gelation-supercritical drying approach. Canola seed meal, a low-value co-product of canola oil extraction, contains cruciferin, napin, and other proteins, with potential in aerogels and other material applications [5, 6]. The focus of the research was on establishing the effect of gelation conditions on the properties of the resulting aerogels.

The structural morphology of the prepared bio-aerogels featured interconnected mesopores, resulting in densities as low as 0.07 g/cm³ and surface areas up to 278 m²/g. The pore size and specific surface area were dependent on the initial protein concentration and the gelation pH. Additionally, the native conformation and bioactivity of the proteins were preserved throughout the process. Calcium ion crosslinking-assisted gelation was found to reduce the volumetric shrinkage of the gel during drying and improve the thermal stability of the resulting bio-aerogel.

This work demonstrated the adaptability of canola protein for creating lightweight, porous materials with enhanced thermal properties, and more generally provided new insights into the assembly of mixtures of proteins into hydrogels and aerogels.

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Effect of gangue content on the compressive strength of hydrogen direct reduced iron ore pellets

Ms Shaira Mendoza[1], Dr Mohammad Nusheh[2], Dr Ben H. Yin[1,3], Prof Chris W. Bumby[1,3]
[1]Robinson Research Institute, Faculty of Engineering, Victoria University of Wellington, Wellington, New Zealand, [2]Hot Lime Labs, Lower Hutt, New Zealand, [3]The MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, Wellington, New Zealand

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Hydrogen direct reduction (H2-DR) of iron ore pellets is a promising alternative ironmaking process with net-zero CO2 emissions. The strength of H2-reduced pellets is an important parameter to ensure that pellets survive processing in a vertical shaft DR furnace. Here we report a study of the evolution of compressive yield strength during H2-DR for pellets formed from two different types of iron ore: low-grade titanomagnetite (TTM) ironsand from New Zealand (NZ) (~59 wt.% Fe) and high purity Swedish magnetite (~72 wt.% Fe). Ex-situ measurements were performed to elucidate the effect of reduction degree, temperature, and gangue on the strength of pellets. Both types of pellets exhibited a significant decrease in compressive yield strength during H2-DR, especially within the initial 30% stage of reduction. The magnetite pellets exhibited a shift from brittle to ductile failure as the reduction progressed, whereas NZ TTM ironsand pellets exhibited brittle failure at all stages of reduction up to 98%. This differing behaviour is attributed to the gangue content and morphology present in each pellet. H2-reduced magnetite pellets exhibited a spongy network of metallic iron interspersed with voids that close under compression, resulting in significant ductile deformation. By contrast, H2-reduced NZ TTM ironsand pellets have extensive inclusions of brittle gangue oxides within the metallic iron, which act to promote crack nucleation and brittle fracture under compression. Our results highlight the important influence of gangue content on the final strength and compressibility of H2-DR pellets.

Synthesis of Magneto-thermal Catalysts for CO2 Hydrogenation

Ms Akshita Mogaveera[1,2], Dr. Chris Bumby[1,2], Dr. Ben Yin[1,2], Dr. Alex Yip[3]
[1]Paihau-Robinson Research Institute, Faculty of Engineering, Victoria University of Wellington, Wellington, New Zealand, [2]The MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, Wellington, New Zealand, [3]Department of Chemical and Process Engineering, Faculty of Engineering, University of Canterbury, Christchurch, New Zealand

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Hydrogenation of CO2 to CH4 is an attractive route to the production of sustainable fuels and chemicals, as CH4 is a well-established industrial feedstock for which conversion and transport infrastructure already exists [1]. However CO2 hydrogenation requires significant heat energy to overcome the activation energy of CO2. Direct magnetic induction heating (MIH) is an attractive heating method that can deliver direct and rapid heating of catalyst particles, minimizing the energy losses and providing precise catalyst temperature control. MIH relies on ferromagnetic hysteresis loss which occurs within magneto-thermal particles when exposed to a high frequency alternating magnetic field [2]. Previously magneto-thermal core-shell catalysts, such as Fe@SiO2@Ni have been reported for the Sabatier reaction [3]. In this work, synthesis of magneto-thermal core-shell catalysts is reported in which using titanomagnetite ironsand has been utilised as the ferromagnetic particle (core), due to its wide availability and uniform chemical composition [4]. These ironsand particles have been coated with a silica shell which then serves as a template for catalyst species deposition, (eg. Cu). The shell also protects the core material from chemical alteration during the CO2 reactions [5]. Silica deposition on ironsand particles has been demonstrated using an MIH-accelerated modified Stober's method [6] which results in direct nucleation of silica on the particle surface. This is followed by in-situ deposition of copper species on the silica shell. The catalyst samples produced will be analysed for CO2 hydrogenation catalysis in later studies.

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Superalkalis as catalysts for carbon dioxide activation

Miss Juliet Nelson[1,2], Dr Celina Sikorska[1,2,3], Professor Nicola Gaston[1,2]
[1]The University of Auckland, Auckland, New Zealand, [2]The MacDiarmid Institute, New Zealand, [3]The University of Gdańsk, , Poland

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Clusters composed of three-atom triangular structure cores, consisting of lithium, aluminum, silver, or gold, were investigated within the superatomic framework. The overall aim of this study was to design novel ligand-protected superatoms that exhibit 'superalkali' characteristics and perform as catalysts for carbon dioxide activation. The chosen ligands were methyl groups ($-CH_3$), phosphine groups ($-PH_3$), and fluorine atoms (-F), covering both electron-donating and electron-accepting characteristics. The study elucidated the relationship between ionization energy, electronic structure, composition, electronic stability, thermodynamic stability, and reactivity of these ligand-protected clusters. Particular focus was given to the effect of the metal core and ligands on electronic stability and the reduction of ionization energies below those of typical alkali metals, thus achieving superalkali behaviour. This DFT study was conducted using the computational chemistry software Gaussian '09 at the MP2/Def2QZVP and CCSD/Def2QZVP levels of theory.

Turning Chrome Shavings Waste into Functional Materials: A Sustainable Approach

Braydon Nikolaison[1], Dr Siew Ling Ong[1], Dr Holger Fiedler[2], Dr Fang Fang[2], Dr Sujay Prabakar[1]
[1]Leather and Shoe Research Association of New Zealand, Palmerston North, New Zealand, [2]GNS Science, Lower Hutt, New Zealand

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Chrome shavings, a by-product of the leather tanning process, are currently landfilled in New Zealand, leading to resource inefficiency and disposal challenges. This study presents a waste-to-value proposition by converting chrome shavings into functional films with potential applications in energy storage systems. The shavings were ball-milled into a fine powder and cast into films, transforming them into a potential high-value material. Characterization by Fourier-transform infrared (FTIR) spectroscopy confirmed that the collagen structure remained intact, evidenced by characteristic amide I, II, and III bands, highlighting the preservation of the characteristic collagen structure. Differential scanning calorimetry (DSC) analysis showed that the films retained the denaturation temperature of chromium-sulfate crosslinked collagen, indicating structural & thermal stability.

Further characterization using Brunauer-Emmett-Teller (BET) surface area measurements revealed a porous microstructure, enhancing the material's suitability for applications requiring high surface area. Electrochemical properties of the film were assessed by impedance spectroscopy to assess ion transport of the films. Results demonstrated that the films exhibit measurable ion conductivity, which varied with different electrolytes. This suggests potential for use in energy storage devices, including batteries, as well as sensors or bioelectronic applications. The findings highlight a sustainable pathway for utilizing leather processing waste, offering both environmental and economic benefits by converting chrome shavings into novel, functional materials.

Tracking Exciton Diffusion in Photoactive and Electronic Frameworks using Ultrafast Spectroscopy

Mr Sam Otter[1]
[1]Victoria University of Wellington, Wellington, New Zealand

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The aims of this presentation and my PhD thesis is to investigate the exact mechanisms involved in exciton diffusion inside of framework materials, such as metal organic frameworks (MOFs) and covalent organic frameworks (COFs).

Framework materials are currently being extensively researched in a wide range of fields due to their permanently porous nature, their ability to be chemically functionalized and to selectively capture gases and compounds. Frameworks have also seen use as photocatalytic materials, specifically in the trapping and converting of green house gases into renewable green fuels.

A key step in using frameworks for photocatalytic applications is understanding how excitons diffuse through framework materials. This work aims to understand how excitons diffuse through framework materials and determining if it's possible to simulate exciton diffusion in current and future frameworks. As the lifetime of an exciton is within the pico-second to nano-second scale, conventional steady-state spectroscopic techniques do not have the temporal resolution to accurately measure their diffusive properties. We instead use ultrafast spectroscopic techniques to accurately measure the exciton diffusion properties of frameworks. We have collected a range of framework families that each contain slight changes in their chemical makeup to understand how these changes effect their exciton diffusion properties. Computational chemistry techniques, such as density functional theory, are used to model and predict the exciton diffusion properties of current and future frameworks.

Perovskite encapsulated metal-organic frameworks

Mr Adrian Owens[1]
[1]Auckland University of Technology, Auckland, New Zealand

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Perovskite encapsulated metal-organic frameworks
The incorporation of caesium lead halide (CLH) quantum dots (QDs) into metal-organic frameworks (MOFs) represents a promising strategy for enhancing the stability and photoluminescent properties of these perovskite materials. This project involves the integration of CLH QDs into four environmentally stable MOFs: HKUST-1, ZIF-8, UiO-66, and UiO-67. The primary objective is to leverage the unique porous structures and host-guest interaction capabilities of these MOFs to stabilize the QDs, thereby preventing degradation and enhancing their optical properties. HKUST-1, ZIF-8, UiO-66, and UiO-67 are selected due to their diverse pore sizes, chemical stability, and potential to form strong host-guest interactions with the QDs. The synthesis involves the sequential deposition of the CLH precursors within the MOF matrices, aiming to create a hybrid material that retains the high photoluminescence quantum yield characteristic of the QDs while benefiting from the structural support and protection offered by the MOFs. The photoluminescent properties of these hybrid materials are analyzed using ultraviolet-visible (UV-vis) spectroscopy, steady-state fluorescence techniques, and time-correlated single-photon counting (TCSPC). These methods enable a comprehensive assessment of the emission characteristics and stability of the QDs when incorporated into the MOFs. The study hypothesizes that the MOF-QD composites will exhibit enhanced photostability and potentially altered emission spectra due to the elimination of capping ligands and to the confinement effects and interactions within the MOF frameworks. This research aims to improve the stability and performance of CLH QDs for photovoltaic applications.

A neuromorphic device for Arithmetic Operations: Influence of Presynaptic Pulsing Scheme on Mathematical Precision

Ms Mousona Pal[1]
[1]Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bengaluru, India

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Modern computers although capable of performing complex tasks, come with inherent limitations arising from their architecture. Following neuromorphic approaches, researchers are developing brain-inspired devices using diverse materials and geometries to replicate neural processes [1,2]. This research is crucial for developing low-energy technologies and future computing systems that go beyond the traditional CMOS and Boolean logic.

The presentation is related to the fabrication and performance of a neuromorphic device consisting of self-formed labyrinthine silver nanostructure capable of exhibiting potentiated states upon electrical activation [3], emulating a bio-synapse with ultralow energy requirement (~ 1 fJ/synapse). The conductance and its retention in the potentiated state both vary linearly with positive and negative polarity pulses exhibiting very low nonlinearity factors. We made several such devices with comparable performances which are indefinitely stable. Leveraging on high linearity, we performed arithmetic operations of summation and subtraction by varying the sequence of feeding positive and negative pulses. These operations yielded highly accurate results; lesser the mixing of polarities higher was the accuracy. Notably, increasing the current compliance increased accuracy, which we attribute to the formation of stronger filaments within the percolation network, thereby enhancing conductance and retention. The treatment was extended to estimation of 'the area under a curve' matching the expected results. Moreover, the device demonstrated a simulation-based image classification accuracy of 94.95%. These features underscore the potential of our scalable device architecture for precise computational applications away from traditional von Neumann architecture.

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An ultrasensitive detection method for ribonuclease H utilizing in vitro transcription of fluorogenic RNA light-up aptamer

Professor Hyun Gyu Park, Jinhwan Lee[1], Soobin Lee[1], Yoonho Nam[1], Hyun Gyu Park[1]
[1]KAIST, Daejeon, South Korea

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Herein, we proposed a label-free method to identify RNase H activity by utilizing in vitro transcription of fluorogenic light-up aptamers. In this work, we employed the specially designed two pivotal components of the hairpin substrate probe (HP) containing an RNA/DNA chimeric stem region and the template probe (TP) as a transcription template, and the RNase H activity was made to lead to the formation of a complete ds T7 promoter. T7 RNA polymerase could then promote in vitro transcription to generate numerous light-up RNA aptamers that result in significant fluorescence enhancements upon binding to the cognate fluorogenic dye. By leveraging this deliberate design principle, we identified RNase H activity ultrasensitively as low as 0.000156 U mL 1 with excellent specificity against non-target enzymes. We further demonstrated that the strategy can also reliably identify RNase H activity in heterogeneous biological samples such as cell lysates, ensuring its robust practical applicability. This work would provide invaluable insight for the development of innovative biosensing systems utilizing in vitro transcription of light-up aptamers, and it could be broadened to construct other assays by appropriately redesigning the HPs.

Stabilized cathode/sulfide electrolyte interface by modified lithium borate coating

Professor Yong Joon Park[1], Mr. Dae Ik Jang[1]
[1]Kyonggi University, Suwon, South Korea

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All-solid-state batteries (ASSBs), which utilize nonflammable sulfide-based solid electrolytes, offer a solution to the safety concerns associated with lithium-ion batteries. ASSBs can also enhance energy density and expand the operating temperature range. However, high reactivity and limited voltage window of sulfide electrolytes pose significant challenges to the interface stability, particularly when contacted with oxide-based cathodes. The deployment of a stable coating layer has proven effective in stabilizing the cathode/sulfide electrolyte interface. Among potential coating materials, lithium borate stands out due to its cost-effectiveness and efficiency in mitigating interfacial reactions. Nevertheless, lithium borate's oxide characteristics create a disparity in the chemical potential of Li+ ions compared to sulfide electrolytes, resulting in an uneven distribution of Li+ ions at the interface. This results in the hindrance Li+ ion's migrations, which deteriorates the electrochemical performance of the cells during charge and discharge cycles. In this study, the lithium borate coating layer was modified with sulfur to overcome this issue through a gaseous reaction involving sulfur elements. This sulfur-modified lithium borate is anticipated to reduce the chemical potential difference of Li+ ions and enhance the electrochemical properties. Various analytical techniques were employed to compare the electrochemical properties of coated and pristine samples, confirming that sulfur modification significantly enhances the performance of the lithium borate coating.

A Computational Investigation into Hydrogen Production on Twisted Molybdenum Disulfide

Miss Kayla Prendergast[1], Mr Christopher Mills[1], Anna Garden[1]
[1]University Of Otago, Dunedin, New Zealand

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Hydrogen is a promising zero-carbon fuel which can be formed using renewable electricity, and when utilising electrolysis the most effective catalysts found so far are all platinum based. Platinum is a rare and expensive metal, attention has shifted to transition metal dichalcogenides, such as monolayer (2D) MoS¬¬2, which are earth abundant and show promising catalytic activity. While currently less effective than platinum-based catalysts, the activity of MoS2 has proven to be highly tuneable by introducing dopants,[1] defects,[2] and supporting materials,[3] which modify the geometric and electronic structure. Very recently, changes in the electronic structure of layered 2D materials have been observed when the layers are twisted relative to each other (see Figure), giving rise to the emerging field of twistronics. Despite growing interest in the topic, little is known about how a twist in supported MoS2 might affect its catalytic activity in the hydrogen evolution reaction. In this work, a systematic computational study will be performed, using density functional theory to calculate the hydrogen evolution activity of twisted, layered MoS2. This will allow the effects of the twist angles on the system to be isolated and examined.

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Development of a hybrid optoelectronic radiation sensor using a Gd2O3 glass scintillator and a TiO2 photoconductor

Dr Marilou Raduban[1,2], Pornnapha Mangthong[3,4], John A. Harrison[5], Michal Kohout[6], Zdeněk Hubička[6], Jiří Olejníček[6], Nattapon Srisittipokakun[3,4], Jakrapong Kaewkhao[3,4]
[1]Unitec Institute of Technology, Auckland, New Zealand, [2]Institute of Laser Engineering, Osaka University, , Japan, [3]Physics Program, Faculty of Science and Technology, Nakhon Pathom Rajabhat University, , Thailand, [4]Center of Excellence in Glass Technology and Materials Science, Nakhon Pathom Rajabhat University, , Thailand, [5]Massey University, , New Zealand, [6]Department of Low Temperature Plasma, Institute of Physics of the Czech Academy of Sciences, , Czech Republic

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Vacuum ultraviolet (VUV) radiation that spans the wavelength range from 200nm to 100nm (6.2eV to 12.4eV) is indispensable in numerous technological applications and scientific research. In recent years, tremendous research has gone into the development of VUV light sources to meet these technological and scientific demands. Development of sensors for this short wavelength region is as crucial. Scintillators are luminescent materials that absorb high energy radiation, converting it into more accessible optical wavelengths through the emission of photons (photoluminenscence/PL) having energies in the UV or visible region. As such, scintillators are the main sensing units in radiation sensors, including VUV. However, a separate photodetector is needed to convert the PL to electrical signals. In this work, we fabricate $48SiO_2$:$25B_2O_3$:$0.5Al_2O_3$:5CaO:$0.5Sb_2O_3$:$10Na_2O$:$9K_2O$:$2Gd_2O_3$ glass scintillators and develop a hybrid optoelectronic VUV sensor by coating the scintillator's surface with a titanium dioxide (TiO_2) thin film. The TiO_2 film with bandgap around 3.2eV serves as a photoconductive sensor that directly converts the PL emission from the Gd_2O_3 scintillator (311nm or 3.99eV) to electrical signals, thereby eliminating the need for an external photodetector. TiO_2 was reactively sputtered in Ar/O_2 atmosphere using DC magnetron sputtering. The effect of heating the Gd_2O_3 scintillator during sputtering of TiO_2 and annealing of the Gd_2O_3-TiO_2 hybrid scintillator post-TiO_2 deposition was investigated. Annealing and heating improved the crystallinity of the TiO_2 photoconductive thin film, increasing the photosensitivity of the film while keeping the photoluminescence properties of the Gd_2O_3 scintillator unchanged. Development of this hybrid scintillator will pave the way towards the miniaturization of scintillators for the detection of high energy radiation.

Isolation and Characterisation of Algal Nanocellulose for Tissue Scaffolding Applications

Miss Janet Reid[1]
[1]University Of Otago, Tauranga, New Zealand

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Nanocellulose is a bio-based nanomaterial with excellent mechanical properties, tailorable chemical characteristics, and good biocompatibility. These qualities make it suitable for the fabrication of cell scaffolding materials, which aim to mimic the structure of native extracellular matrix to allow for effective tissue regeneration. Marine algae present a novel source of nanocellulose, which has a higher crystallinity index and wider fibril morphology in comparison to material derived from terrestrial plant sources. Cellulose nanofibrils (CNFs) were isolated from four commercially important New Zealand seaweed species (Ulva australis, Ecklonia radiata, Lessonia variegata, and a Gelidium sp.) after a single pass through a high-pressure homogeniser. Scanning electron microscopy showed that algal CNFs formed a dense network with an average fibril diameter of 20nm. Thermogravimetric analysis revealed that the thermal stability of the nanocellulose differed between species, and CNFs derived from the two kelp species had a degradation temperature higher than that of commercially available microcrystalline cellulose (365°C vs 336°C, respectively). Nanocellulose biocompatibility was assessed using an MTT assay, which showed no indication of toxicity against human keratinocyte cells even at the highest concentration tested (1mg/mL). Finally, keratinocyte cells were cultured on CNF sheets for two days, which indicated that cells attached to the sheets but did not proliferate into monolayers. These results indicate that CNFs isolated from algae may be suitable for cell scaffolding applications, due to their biocompatibility and unique physical characteristics.

A Comprehensive Guide to Exploring Electrochemical Nitrogen Reduction in Model Catalysts

Mr Zulfitri Rosli[1,2,3], Dr Siriluck Tesana[1], Prof Peng Cao[2,3], Dr Prasanth Gupta[1,3]
[1]GNS Science, New Zealand, [2]University of Auckland, , New Zealand, [3]The MacDiarmid Institute of Advanced Materials and Nanotechnology, , New Zealand

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Producing ammonia through the direct electrochemical nitrogen reduction reaction (eNRR) offers a promising route for developing green fertilizers and zero-carbon energy vectors. However, the field faces significant challenges, including widespread ammonia contamination and the low production rates of eNRR systems, often leading to false positives in ammonia detection. Stringent protocols have been established to eliminate these false positives and ensure reliable eNRR performance measurements, though these protocols are often incompatible with fundamental investigations using model thin film catalysts.

In this work, we adapt these rigorous eNRR protocols to measure the performance of transition metal nitride catalysts developed through ion implantation. Detailed characterisations were conducted to correlate their structural properties with electrocatalytic performance. Using the GNS experimental test station as a case study, we present a rational and reliable method for measuring and validating eNRR performance, specifically focusing on production rate and Faradaic efficiency. Our approach addresses various sources of ammonia/nitrogen compound contamination, the impact of random errors, and the accuracy of popular ammonia measurement techniques, including ion chromatography and colorimetry. By applying these stringent protocols to our model catalysts, we demonstrate their applicability and assess the confidence level of the results. Our findings indicate that most of these catalysts fail to produce statistically significant ammonia, with the potential exception of one nitride where genuine eNRR may be detected.

Quinone-containing Molecular Catalysts for Photocatalytic Hydrogen Generation

Miss Leah Sammon[1], Dr. Chris Fitchett[1]
[1]University Of Canterbury, Christchurch, New Zealand

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

As energy consumption and related greenhouse gas emissions reach record levels, efficient routes to H_2 production are sought after for use as carbon-free fuel. However, 99.3% of current methods come from non-renewable energy sources and generate significant CO_2 emissions.[1]

Artificial photosynthesis has long been a research target in combatting this since its energy source – solar light – is abundant and renewable. By mimicking the highly organised architectures utilised by natural photosynthetic systems, improvements can be made on conventional hydrogen-evolution reaction (HER) photocatalysts.[2]

Photocatalytic HER requires multiple photon equivalents of energy captured by a light-harvesting unit, and a catalytic centre.[3] Accumulating this energy as reductive potential is a key issue in the development of such catalysts. Prolonging the lifetime of this energy by charge separation is a method used by natural photosynthetic systems that increases the efficiency of this process. Quinone moieties are often utilised for this purpose owing to their stability and the reversibility of the redox couple.[4]

Previous research has found that quinone-containing ruthenium(II) complexes can successfully accumulate light energy in the quinone moiety as reduction potential.[5] Inspired by these results, this work aims to explore methods for including quinone molecules into supramolecular architectures desirable for light harvesting and successfully characterise their catalytic performance.

This work also seeks to introduce these complexes into covalent organic frameworks, with the intention of utilising their desirable physical characteristics to generate photocatalysts that are efficient, stable, and tuneable.[6]

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Ruthenium-gold cluster catalysts for CO2 reduction

Mr Michelangelo Santos[1]
[1]University Of Canterbury, Christchurch, New Zealand

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Ultrasmall-sized, atomically precise metal clusters show distinct physical and chemical properties compared to their bulk metal counterparts [1]. As the number of atoms in the cluster core decreases, the continuous band of the metallic state shifts towards quantised energy levels of a non-metallic state, leading to unique geometric and quantised electronic structures [2]. The high surface area-to-volume ratios of clusters increase atom utilisation in catalysis [3]. Industrial processes relying on fossil fuels emit CO_2, exacerbating the challenges of climate change. Removing CO_2 from the atmosphere provides an opportunity to convert CO_2 into different chemicals. Work by the Golovko group has shown that monometallic gold clusters catalyse CO_2 electro-reduction to CO with high selectivity [4]. Such studies have been complemented with synchrotron-based spectroscopy (XAS) to study how clusters evolve during catalysis [5]. However, introducing heteroatoms into a metal core can tune the structure and surface composition of metal clusters [3]. An inert polarity within heterometallic bonds could direct the selectivity of substrate-catalyst interactions to enhance catalytic activity [6]. Recently, Hudson R. J. showed that $AuRu_3$ clusters on anatase TiO_2 improve the efficiency of CO_2 photo-reduction than ruthenium-based clusters [7]. This presentation highlights the studies on Ru-Au mixed-metal clusters as potential catalysts for CO_2 reduction, including the formation and characterisation of a novel "Ru_3Au_2" cluster exhibiting a trigonal bipyramidal arrangement with both Au atoms above and below the Ru_3 metal core. Notably, the crystal structure of Ru_3Au_2 has been resolved and XAS studies were performed with said cluster.

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Investigating the Thermal and Structural Properties of 2D Low Temperature Melting Metals

Miss Caitlin Scott[1]
[1]University Of Auckland, Auckland, New Zealand

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

With the successful exfoliation of a number of 2D structures beginning with graphene and more recently stanene, bismuthene and gallenene, discoveries of their potential applications as topological insulators or energy storing devices has increased the interest in their theoretical properties [2].

Previous studies using ab initio molecular dynamics (AIMD) have shown that the melting temperature of gallenene varies significantly as a function of the number of layers in the 2D structure. These studies also showed a change in solid phase before melting where 2 to 6 layers were analysed [1] [3].

In this work we investigate the thermal stability of 2D bismuth and tin structures using ab initio molecular dynamics to calculate the melting temperatures for different thicknesses. This analysis will have implications for the utility of these 2D materials in the future.

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Detection of Food Freshness Using Biodegradable Composite Polymer

Miss San San Shen[1], Mr Yu Sun[1], Mr Xue Jun Li[1]
[1]Department of Electrical and Electronic Engineering, Auckland University Of Technology, Auckland, New Zealand

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

The concentration of ammonia gas is often used as an indicator of the freshness of high-protein food, like meat and milk. However, currently used sensor systems, like semiconducting metal oxides, polyaniline etc., tend to be toxic in food-related environments, which could lead to potential food contamination. Therefore, it is desired to design and develop a non-toxic and safe sensor that is biodegradable. Soy Protein Isolate (SPI) and purple cabbage anthocyanins (PCA) are identified as promising candidates because of their distinct properties. In particular, Soy Protein Isolate (SPI) is a remarkable natural polymer with abundant hydrogen bonds and awe bonds; purple cabbage anthocyanins serve as remarkable natural indicators due to their safety, non-toxicity, and sensitivity to environmental pH. Their biodegradable nature ensures they don't cause end-of-life pollution, making them an environmentally friendly solution for food safety monitoring. Based on this consideration, by integrating specific sensing elements (e.g., PCA) into biodegradable polymers (e.g., SPI), we designed a SPI/Na2SO4/PCA sensor film capable of changing colours in response to pH variations, which can be observed with the naked eye. Experimental results showed that the colour of the film changes from green to red when pasteurized milk is no longer fresh. Moreover, this study demonstrated that the film's colour high stability duration exceeds five days regardless of whether under light exposure or in the absence of light. These findings underscore the sensors' practical potential in food safety, highlighting their reliability and effectiveness in detecting ammonia, which is considered as a key marker of food spoilage.

Innovative Exosome Isolation Technology Utilizing a Sequential Combination of Charge-Based Filtration, Tangential Flow Filtration, and Lipoprotein-Specific Adsorption

SoYoung Jeon[1], YongWoo Kim[1], Professor SungSoo Na[1], Dr Sehyun Shin[1]
[1]Korea University, Seoul, South Korea

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

This study introduces an innovative hybrid EV extraction technology by combining the charge-based exosome separation technology, ExoFilter, with lipoprotein-specific adsorption filter technology and integrating it with Tangential Flow Filtration (TFF), a technology that excludes nanoparticles below a certain size. Traditional technologies often face significant challenges in effectively removing impurities and processing large sample volumes. The need to overcome these limitations has driven the development of this advanced methodology, which addresses these constraints by offering improved purity and scalability. ExoFilter, an ion-exchange based technology, was recently developed to process negatively charged EVs from small sample volumes to liter-scale samples. TFF, widely used for its unique ability to concentrate samples by excluding nanoparticles below a specific size, when combined with charge-based ExoFilter technology, achieved unexpectedly high recovery rates and high purity through iterative flow processes. Additionally, by incorporating a filter process with an Apop-B-specific aptamer, a surface marker of lipoproteins, the previously obtained high-purity extracts were further refined to ultra-high purity without reducing recovery rates. This series of integrated processes retained the individual technical advantages, resulting in remarkable purity improvement and a synergistic effect that more than doubled the existing recovery rates. This represents a significant technological advancement in the extraction technology by efficiently removing lipoproteins, which are difficult to eliminate with conventional methods. The combined technology of each filter, scalable from small blood samples to hundreds of liters of culture medium, presents a new method for efficiently obtaining high-quality exosomes for various biological and medical applications.

Optimized Extraction Methods for Purifying Bio-Synthesized Indigo from Bacterial Residue and Contaminants

Professor Younga Son[1], Dr Ramalingam Manivannan[1], Dr. Kalian Prabakaran[1]
[1]Chungnam National University, Daejeon, South Korea

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Bio-dyes constitute a class of natural dyes derived from renewable and sustainable sources, offering an eco-friendly alternative to traditional synthetic dyes. Indigo, a prominent bio-dye, is an organic compound renowned for its intense blue color. The development of an environmentally sustainable and highly efficient biocatalyst for the production of indigo is critical, given the increasing demand for blue colorants. During batch fermentation, E. coli has demonstrated an improved ability to withstand the cytotoxic effects of elevated indigo concentrations, maintaining plasmid stability throughout the process. The subsequent isolation of indigo from the E. coli culture was achieved through a series of solvent extraction techniques designed to selectively isolate the target compound from the bacterial matrix. The bio-indigo was further purified using a combination of ultrasonication, centrifugation, and filtration techniques. The structural integrity and purity of the bio-indigo were confirmed through comprehensive analysis using NMR spectroscopy and UV-visible spectroscopic methods.

High-performance bipolar membranes for efficient direct seawater electrolysis

Ms. Hyeong-Bee Song[1], Ms. Ji-Hyeon Lee[1], Professor Moon-Sung Kang[1]
[1]Sangmyung University, Cheonan-si, South Korea

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Hydrogen is a crucial energy carrier for the development and maintenance of a low-carbon economy through sustainable energy generation. Among various methods for producing hydrogen, water electrolysis is considered the most efficient. To electrolyze water efficiently, excellent electroactive catalysts and ion-exchange membranes that can efficiently separate the anode and cathode are required. Recently, direct seawater electrolysis (DSWE), which produces hydrogen by decomposing seawater, has attracted attention in terms of economy and efficiency [1]. To mitigate the formation of inorganic precipitates from multivalent ions present in seawater, typically, bipolar membranes (BPMs) with acid-base generating properties and porous electrodes are introduced in a zero-gap configuration [2]. The BPM can suppress the formation of inorganic precipitates due to multivalent ions in the DSWE process and enable efficient OER and HER [3]. In this study, a highly durable BPM suitable for the high-current DSWE was developed. In particular, the water-splitting performance of the BPM was significantly improved by applying catalysts based on graphene oxide (GO) and metal particles. In addition, the membrane structure and fabrication method for improving the interfacial durability of the BPM were proposed. The fabricated BPM showed excellent water-splitting performance and mechanical strength compared to commercial membranes. In addition, when applied to the DSWE process, it showed good stability without interfacial detachment under high-current operating conditions. This work was supported by NRF grants funded by the Government of Korea (MEST) (NRF-2022M3C1A3081178 and NRF-2022M3H4A4097521).

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Optogenetic and chemogenetic modulation of cognitive function in mice

Professor Kyoungho Suk[1], Jae-Hong Kim[1], Michiko Nakamura[1], Professor Kwon Moo Park[1], Maan-Gee Lee[1], Professor Il-Sung Jang[1]
[1]Kyungpook National University, Daegu, South Korea

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Previous studies have shown the importance of astrocytes in memory and other cognitive functions. However, reactive astrocytes are associated with neuroinflammation and cognitive decline in diverse neuropathologies. Optogenetics and chemogenetics are powerful tools that enable precise control and manipulation of specific neural circuits within the brain. Optogenetics utilizes a light-sensitive ion channel expressed in targeted cells, allowing for control with pulses of light. For chemogenetics, the designer receptors exclusively activated by designer drugs (DREADDs) are expressed in specific target cells, and a designer ligand is used to induce activation or inhibition of target cells. We used optogenetic and chemogenetic tools to identify the crucial roles of the hippocampal CA1 astrocytes in cognitive decline. Our results showed that repeated optogenetic stimulation of the hippocampal CA1 astrocytes induced cognitive impairment in mice and decreased synaptic long-term potentiation (LTP), which was accompanied by the appearance of inflammatory astrocytes. Reactive astrocytes mediated neuroinflammation and induced cognitive impairment by decreasing the LTP. Sustained chemogenetic stimulation of hippocampal astrocytes provided similar results. Conversely, these phenomena were attenuated by a metabolic inhibitor of astrocytes. Fiber photometry using GCaMP revealed a high level of hippocampal astrocyte activation in the neuroinflammation model. Our findings suggest that reactive astrocytes in the hippocampus are sufficient and required to induce cognitive decline through synaptic modulation. This abnormal glial–neuron interaction may contribute to the pathogenesis of cognitive disturbances in neuroinflammation-associated brain conditions. Thus, targeting astrocyte pathways could offer new therapeutic approaches to treat cognitive alterations in brain disorders.

Nanostructure, Morphology, and Electrochemistry of Degradable Oligo(3-hexylthiophene) Grafted onto Poly(caprolactone)

Ms Yuhka Uda[1,2], Dr Eddie Wai Chi Chan[1,2], Dr Nigel Kirby[3], Mr Timothy Lambden[4], Prof. David Barker[1,2], Prof. Jadranka Travas-Sejdic[1,2]
[1]MacDiarmid Institute for Advanced Material and Technology, Wellington, New Zealand, [2]Centre for Innovative Materials for Health, School of Chemical Sciences, The University of Auckland, Auckland, New Zealand, [3]Australia's Nuclear Science and Technology Organisation, Melbourne, Australia, [4]Department of Materials Science & Metallurgy, , United Kingdom

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To mitigate the issues surrounding e-wastes, a novel CP-based material, oligo(3-hexylthiophene) graft copolymer, termed P(CL-co-AVL)-g-O3HT, was developed as a conductive and degradable material for potential applications in transient devices.1 Building on this work, a comprehensive analysis on the structural, electrochemical, and optical properties were conducted to understand the relationship between the properties and the molecular design (oligomer length, grafting density), as well as the processing conditions (annealing, solvent-treatment). Nine graft copolymers were prepared with different combinations of oligomer lengths (n= 15, 30, and 40 mers) and grafting densities (CL:AVL = 9:1, 14:1, and 25:1). Graft copolymers with long O3HT lengths (n=30, 40 mers) exhibited well-defined crystalline domains of both O3HT and P(CL-co-AVL), as observed by Small-angle X-ray Diffraction and Scanning Electron Diffraction. Cyclic voltammetry and In-situ UV-vis spectroscopy analysis suggested good electrochemical and electrochromic properties of graft copolymers with well-organised O3HT branches. P(CL-co-AVL)-HD-g-O3HT-30 (CL:AVL = 9:1, n=30) had the optimal O3HT microstructural features and film-forming ability, achieving a conductivity of 3.1±0.1 mS/cm. Annealing at 40 °C was found to assist the formation of the tightly packed, thermodynamically-favoured O3HT stacking (Form II polymorph) and severely disrupt the crystalline domains of P(CL-co-AVL). Small volumes of acetonitrile were found to induce pre-aggregation of polymer chains in solution, assisting the formation π-π stacks and the Form II polymorph. The improved crystalline quality led to P(CL-co-AVL)-HD-g-O3HT-30 with electrochemical oxidation at a lower potential.

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The plasma-assisted thermal catalytic process for CO2 conversion

Dr Settakorn Upasen[1], Dr Soipatta Soisuwan[1,2], Mrs. Sorawe Setasuban[1], Mrs. Wanida Malaphum[1], Dr. Héctor Morillas[3], Dr. Joongjai Panpranot[4]
[1]Department of Chemical Engineering, Engineering Faculty, Burapha University, Saensuk Sub-district, Muang District, Chonburi, 20130, Thailand, [2]Interdisciplinary Center for Decarbonisation and Green Energy, Faculty of Engineering, Burapha University, Saensuk Sub-district, Muang District, Chonburi, 20130, Thailand, [3]Department of Analytical Chemistry, Faculty of Science and Technology, University of the Basque Country (UPV/EHU), P.O. Box 644, 48080 Bilbao, Basque Country, Spain, [4]Center of Excellence on Catalysis and Catalytic Reaction Engineering, Department of Chemical Engineering, Faculty of Engineering, Chulalongkorn University, Bangkok, 10330, Thailand

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In this study, the thermal and plasma-assisted thermal catalytic processes were performed to convert CO_2 into CH_4 fuel gas under various conditions. The aim is to search for the potential of the methanation reaction at low temperatures. A series of Ni-xCeO_2/LTA-5A and Co-xCeO_2/LTA-5A catalysts with an active metal content (Ni and Co) of 15 wt.% and different CeO_2 doping (0-15 wt.%) were employed and prepared by a conventional dry impregnation method. Various analytical techniques, including SEM-EDX and BET methods, were used to examine the catalyst surface and bulk characteristics. The temperature of the methanation reaction for the conventional thermal-catalytic process varied from 100 to 400°C, and the plasma-assisted thermal-catalytic was operated at 25-150°C. The result of the thermal-catalytic process for all prepared catalysts showed that increasing temperature could increase the activity of CO_2 conversion and the CH_4 productivity – mainly operated at 400°C with a CO_2 conversion of 94-99% and CH_4 selectivity 93-95%. The effect of CeO_2 amount addition into Ni-based/LTA-5 catalysts could promote and stabilize the catalytic performance—the appropriate amount of 5 wt.% CeO_2. For the plasma-assisted thermal catalytic process, the plasma electrical potential significantly affected the low-temperature (below 150°C) methanation reaction although its activity and productivity remained low. The nickel-based metal catalyst was more active than cobalt metal for the low-temperature plasma-assisted thermal catalytic process.

Tuning magnetic properties in rare-earth nitrides: exploring GdNdN for compensation points

Ms Kiri Van Koughnet[1,3], Dr Will Holmes-Hewett[2,3], Dr Joe Trodahl[1], Dr Ben Ruck[1,3]
[1]School of Chemical and Physical Sciences, Victoria University of Wellington, Wellington, New Zealand, [2]Robinson Research Institute, Victoria University of Wellington, Wellington, New Zealand, [3]The MacDiarmid Institute for Advanced Materials and Nanotechnology, Wellington, New Zealand

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As the only series of intrinsic ferromagnetic semiconductors, the rare-earth nitrides offer a host of opportunities for exploration in both fundamental science and spintronics applications. Properties such as saturation magnetization, coercivity, and angular momentum can be tailored through the choice of rare-earth ions, leveraging their strong spin-orbit interaction and the varied fillings of their 4f shells. The chemical similarity of the rare-earths and the shared structure of the nitrides opens possibilities for continuous tunability of the magnetic properties in solid solutions [1]. This control over magnetic properties is particularly advantageous for spintronic applications, including cryogenic data storage essential for future superconducting and quantum computing technologies [2,3,4]. These solid solutions have already shown promise in a non-volatile cryogenic magnetic memory element [4]. We report the early studies of the next promising composition, GdxNd1-xN. Here, a spin-only ferromagnet (GdN) is paired with an orbital-dominant ferromagnet (NdN) which suggests the search for a net zero magnetic moment compensation point and a net zero angular momentum compensation point. Both of these compensation points are fundamentally and technologically important, their realization will enable the formation of new low-energy devices, magnetic fringe field free spin currents and enable the detailed study of the spin-orbit physics central to rare-earth materials.

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Tailoring Functional Properties of Perovskite Oxides Using Anisotropic Epitaxy

Mr David Walker[1], Dr Daniel Sando[1]
[1]University Of Canterbury, Christchurch, New Zealand

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

The quest for advanced, eco-friendly, and cost-effective materials is driving research into novel physical properties of complex materials. Perovskite oxides (ABO_3), with their intriguing electrical, magnetic, and catalytic properties, are prime candidates for next-generation devices and energy solutions [1,2]. This poster aims to shed light on how using anisotropic epitaxy in depositing thin films by pulsed laser deposition can engineer the functional properties of perovskite oxides, specifically lanthanum strontium manganite ($La_{1-x}Sr_xMnO_3$ or LSMO), by controlling crystal growth through substrate miscut angles. Anisotropic epitaxy offers a unique approach to manipulating strain and crystal lattice orientation, thereby tuning material properties such as electrical transport and magnetism [3].

This presentation will summarise our preliminary efforts in tailoring the transport and magnetic response of LSMO thin films. The research presented involves the growth of epitaxial LSMO thin films on substrates with varying lattice constants and miscut angles using pulsed laser deposition. The structural integrity and surface morphology of the films is characterised through x-ray diffraction and atomic force microscopy. Subsequent analysis will focus on the impact of strain and orientation on the electrical and magnetic properties of LSMO, including resistivity, magnetoresistance, and phase transitions. The findings aim to advance the understanding of how anisotropic epitaxy can be utilised to tailor perovskite-based materials for applications in spintronics and energy technologies [4]. The study's outcomes are expected to provide a framework for designing high-performance materials and devices, highlighting the potential of anisotropic epitaxy in material science.

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Study on the preparation of CO2 based monomers via cyclization of Glycidyl Methacrylate and CO2 and its polymerization

Professor Cheng-Chien Wang[1]
[1]Southern Taiwan University of Science and Technology, Tainan, Taiwan

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Carbon dioxide (CO2) capture and utilization have emerged as imperative research avenues in response to global climate change concerns. This study focuses on the synthesis of a CO2-based monomer, 2-oxo-1,3-dioxolane-4-yl) methyl methacrylate (GCMA), via the esterification of glycidyl methacrylate (GMA) monomer with CO2. The resultant CO2-based polymer material was prepared GCMA via radical polymerization. GCMA was characterized using FTIR and 1H NMR spectra. The FTIR spectrum of GCMA exhibited characteristic peaks of cyclic carbonate group at 1790 cm−1, 1089 cm−1, and 1048 cm−1, while the peaks at 1719 cm−1 and 1152 cm−1 were attributed to the -C=O and -C-O of ester group. Remarkably, the characteristic peak of the vinyl group (-C=C-) at 1637 cm−1 remained even after cyclic carbonatization. Additionally, the intensity of chemical shifts for the oxirane groups of GMA at 3.23, 2.83, and 2.65 ppm significantly reduced to minimal signals, while the chemical shifts for the cyclic carbonate group at 5.0 ppm and 4.3 – 4.6 ppm were observed in the 1H NMR spectrum. Furthermore, the area and chemical shift for the vinyl group at 6.2 ppm and 5.6 ppm remained unchanged after cyclic carbonatization, indicating the successful conversion of GMA and CO2 into GCMA. Subsequently, the GCMA monomer and acrylate monomer were initiated by K2S2O8 via emulsion polymerization, resulting in the successful preparation of GCMA copolymer latex. The glass transition temperature (Tg) of GCMA copolymers can be adjusted by varying the composition of acrylate monomers and holds promise for future applications in the low-carbon coating industry.

Wicking dynamics of two-ply channels in porous medium-based microfluidic devices

Yung-Ching Wang[1]
[1]National Taiwan University, Taipei, Taiwan

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Microfluidic paper-based analytical devices (µPADs) offer significant advantages such as minimal reagent consumption, portability, and user-friendly operation, making them highly suitable for applications in environmental monitoring, including wastewater and pollutant detection. However, the slow wicking of liquids in paper (porous) channels limits their efficiency and the achievable length of channels, posing challenges for real-time analysis in extended applications.

In this study, we employ many-body dissipative particle dynamics (MDPD) simulations to investigate capillary flow in two-ply channels, with a focus on optimizing their use in environmental applications. We systematically explore the effects of gap width, porosity, and thickness of porous media on imbibition rates, factors critical for improving fluid transport in µPADs designed for pollutant detection. Additionally, we compare the imbibition processes in single-ply channels with varying porosity and thickness to better understand the dynamics. By analyzing the distribution and evolution of the liquid front (penetration length) across the device, which is not captured by modified Washburn's equations, we provide insights into enhancing the performance of µPADs for environmental monitoring.

Our findings reveal that introducing a gap in the two-ply channel leads to a significant increase in the imbibition rate—by at least four times compared to single-ply channels. This enhancement is primarily due to side-imbibition from the gap, improving fluid transport into the porous sheet. These results have important implications for the design of advanced materials in µPADs, particularly for applications in wastewater and pollutant treatment.

Raman spectroscopy to investigate historic paint samples.

Miss Carlie Watt[1,2,3], Genevieve Silvester[4], Emily Fryer[5], Hatesa Seumanutafa[5], Dr Cushla M. McGoverin[1,2]
[1]Department of Physics, The University of Auckland, Auckland 1010, New Zealand, [2]Te Whai Ao — Dodd-Walls Centre for Photonic and Quantum Technologies, The University of Auckland, , New Zealand, [3]Te Mana Tangata Whakawhanake — MacDiarmid Institute for Advanced Materials and Nanotechnology, The University of Auckland, , New Zealand, [4]Conservation Research Centre, Auckland Art Gallery Toi O Tamaki, Auckland 1141, New Zealand, [5]The Canterbury Museum, Christchurch 8013, New Zealand

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Scientific analysis is a valuable tool for informing conservation and cultural heritage studies. Given the fragility, and historical and cultural significance of many works, information-rich, and non-invasive or minimally invasive analytical techniques have been increasingly used. Raman spectroscopy has been increasingly used, as seen by the growth in publications using Raman spectroscopy to study paintings and cultural objects in the past twenty years.(1) Raman is especially useful for identifying colourants, both mineral (e.g., red lead, lead white) and organic (e.g., carotenoids). However, employing scientific analysis in a cultural heritage environment requires additional considerations beyond experimental technical parameters. It is important to be aware of the history of the item being investigated, operating with consideration and awareness of its cultural significance.

Hau Te Ananui o Tangaroa is a whare whakairo cared for by Canterbury Museum. As part of a larger conservation project for its upcoming installation. Raman spectroscopy was used in conjunction with scanning electron microscopy with energy dispersive X-ray spectroscopy (SEM-EDX) to investigate paint on the whare whakairo. The scope of this conference submission will limit itself to the discussing Raman spectroscopic measurements. Paint samples for scientific analysis were taken from multiple heke (rafter), heke tipi (gable end rafters), and pou (carved wall panels). The samples were examined to identify colourants and paint media used on the whare and determine whether a distinction could be made between the materials used on different parts of the whare. A variety of colours were sampled, including white, red, black, blue, and green paint. Raman spectra suggested the presence of red lead and Prussian blue.

Overall, this scientific research aims to investigate the paint used historically. This information will assist conservation decision making through a better understanding of the paint stratigraphy on different parts of the whare. Finally, this research has served as valuable learning experience for the presenting author in undertaking scientific analysis in a cultural heritage environment.

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Synthesis and properties of wool keratin-polysaccharide composite hydrogels

Mr Junfeng Wu[1], Dr Mark Staiger[1], Dr Santanu Deb-Choudhury[2], Dr Pramod Gopal[3]
[1]Department of Mechanical Engineering, University of Canterbury, Christchurch, New Zealand, [2]Proteins and Metabolites Team, AgResearch Ltd, Lincoln Research Centre, Christchurch, New Zealand, [3]The New Zealand Institute for Plant and Food Research Ltd, Palmerston North, New Zealand

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Background: Wool keratin is a biocompatible and biodegradable material, and keratin-based hydrogels show great potential in drug delivery and tissue engineering. However, the poor mechanical properties and brittle structure of keratin hydrogels hinder their use in various applications. Polysaccharides such as inulin and pectin, noted for their stabilising roles and unique rheological properties, can enhance the stability and functionality of hydrogels.

Objective: The present study aims to design hybrid hydrogels that incorporate polysaccharides into keratin gels and to investigate the gel properties and interaction mechanisms between the polysaccharides and keratin within the gel matrix. The goal in the present work is to investigate the synthesis and properties of novel keratin-inulin and keratin-pectin composite hydrogels.

Method: Wool keratin was extracted from wool fibres using a reduction method. Inulin and pectin were selected as polysaccharides to enhance the hydrogel network. The hydrogels were prepared by blending wool keratin with varying ratios of inulin or pectin. The extracted keratin content was fixed at 5% w/v, and different concentrations of polysaccharides (0%, 1%, 3%, and 5% w/v) were added at room temperature to induce gel formation by adjusting the pH. The microstructure, gel water-holding capacity, rheological properties, and mechanical properties of the hydrogels were determined. Additionally, FTIR spectra and Raman spectroscopy were employed to analyse the molecular features and correlations between keratin and polysaccharides, verifying the impact of biopolymer structure on gel properties.

Results and Discussion: Microstructural analysis showed that keratin hydrogels incorporating inulin or pectin exhibited a dense and well-organized network, leading to a more homogeneous and compact gel structure. The hybrid hydrogels demonstrated enhanced water-holding capacity, improved texture profiles, and favourable rheological behaviour, while effectively limiting water fluidity. The results of FTIR spectra and Raman spectroscopy suggested that during acid-induced gelation, the secondary structure of keratin changes, leading to a higher interaction of the polysaccharides with keratin. Specifically, hydrogen bonds between polysaccharides and keratin strengthened, and improving the gel properties.

Conclusion: The results indicated that adding inulin or pectin could strengthen the molecular bonding of keratin and the gel network structure, thus improving the keratin gel properties. The hybrid hydrogels show potential for further development and application in various biomedical fields.

Keywords: Wool keratin, polysaccharide, hydrogel, biomedical applications

Symmetry Engineering Novel Domain Structures in Barium Titanate Thin Films

Mr Tianyuan Wu[1], Prof. Catherine Bishop[1], Dr. Daniel Sando[1]
[1]University Of Canterbury, Christchurch, New Zealand

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Perovskite materials, such as barium titanate ($BaTiO_3$ - BTO), are central to a wide range of applications, including sensors, actuators, and memory devices, due to their tuneable ferroelectric and piezoelectric properties [1]. Traditionally, the performance of BTO thin films has been enhanced through doping and epitaxial strain [2-4].

This study explores a novel approach by depositing BTO thin films on strontium titanate (STO) substrates with large miscuts, where the substrate induces anisotropic strain on the films, potentially leading to enhanced material properties.

Both theoretical simulations with phase field modelling [5] and experiments will be employed. Equations that account for the asymmetric epitaxy conditions will be incorporated into traditional phase field models. This modelling will predict the behaviour of ferroelectric domains and other material properties.

Experimentally, BTO will be grown on STO substrates, including the (001) orientation as a control, and (102) and (103) orientations, which have 26 and 18 degree miscuts respectively. The films are grown by pulsed laser deposition , followed by atomic force microscopy to assess surface morphology and roughness, and X-ray diffraction to identify the phases, crystal structure, crystallinity, and film thickness. Piezoresponse force microscopy will characterise the domain structure.

The findings could pave the way for the development of more efficient perovskite-based devices, as well as provide valuable insight into possible new ferroelectric switching paths in anisotropic-strain engineered films, inspiring future research into the use of substrate engineering as a tool for strain control in thin film technologies.

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The synthesis and luminescence properties of ZnO-doped Y2O3 ceramics

Miss Yu-Hui Xue[1], Mr Jiann-Shing Lee[1]
[1]Department of Applied Physics, National Pingtung University, Taiwan, Pingtung, Taiwan, [2]Department of Applied Physics, National Pingtung University, Taiwan, Pingtung, Taiwan

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

The study explores the luminescence properties of ZnO-doped Y2O3 ceramics prepared by using a wet chemical method. The Y2O3 was chosen as the matrix due to its excellent heat and corrosion resistance, which is suitable for use in harsh environments. However, pure Y2O3 only emits weak light, so it is usually necessary to introduce optically active activators (ZnO) to make it an efficient luminescent material. To fabricate the ZnO-doped Y2O3 powder, yttrium nitrate and zinc acetate were used in the study as the precursors of Y2O3 and ZnO, respectively. These as-prepared samples were characterized by XRD, TEM, BET, zeta potential analyzer, and PL (photoluminescence). After soaking in Zn2+ solution, the synthetic Y2O3 powder pre-treated at 900°C for 2 hours exhibited a stronger green luminescence band with a maximum around 535 nm in the work. The experimental results also revealed that the pH value and Zn2+ concentration when synthesizing ZnO-doped Y2O3 ceramic significantly affect its PL intensity. As is clear from experimental data, the luminescent properties of these powders depend on the content of various defects in the nanoscale crystal. The study shows that the ZnO-doped Y2O3 ceramics can be fabricated through a facile wet method, and they exhibit excellent luminescence properties and potential for optical components.

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Proteolytic reaction-based electrochemical biosensor chip for point-of-care testing

Professor Haesik Yang[1]
[1]Pusan National University, Busan, South Korea

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

Electrochemical protease biosensors are well-suited for simple and quantitative point-of-care testing. However, there has been limited development of versatile chip formats similar to lateral-flow and glucose test strips for electrochemical proteases biosensors. This paper presents a versatile electrochemical biosensor chip for the wash-free and sensitive detection of proteases. The chip comprises (i) a reaction well, (ii) micropatterned electrodes on a glass substrate, and (iii) target protease-dependent filter paper. All (bio)chemicals required for the proteolytic reaction and signal amplification were predried on filter paper, which was then placed inside the reaction well. Upon injecting the sample solution into the reaction well, most of the dried (bio)chemicals dissolved rapidly. Wash-free and sensitive protease detection was achieved using electrochemical-enzymatic (EN) redox cycling of a redox-active species (4-amino-1-naphthol, AN) liberated from a peptide substrate through a rapid proteolytic reaction. The EN redox cycling involves a working electrode, AN, glucose dehydrogenase, and glucose. To enhance dissolvability and stability, (bio)chemicals were dried using a surfactant and stabilizer and stored at 4 °C with vacuum sealing. To minimize the effect of background variation among the different samples, a high concentration of glucose (200 mM) was used, and the difference between the two charge values obtained before and after the incubation period was measured. The biosensor chips successfully detected three proteases: thrombin, leucine aminopeptidase (LAP), and 3CL protease from coronavirus SARS-CoV-2 (Mpro). The detection limits of thrombin in artificial serum, Mpro in artificial saliva, and LAP in human serum were approximately 100, 100 pg/mL, and 8 U/L, respectively.

Development of smart wound-healing device based on conducting polymers

Miss Kourtney Yang[1]
[1]University Of Auckland, Auckland, New Zealand

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In recent years, smart, integrated conductive polymer wound healing devices have become of particular interest, combining the benefits of multi-functional dressings, precisely controlled drug release, biosensing, stimulation and real-time monitoring of wound status.

We recently reported a poly(3,4-ethylenedioxythiophene) (PEDOT)-based platform that utilises the EDOT-thioacetate derivative (EDOTSAc) to provide a thiol functionality that is capable of electrochemical and reversible conjugation of various (bio)molecules. This has enabled the capture and release of small and bio-molecules, such as 2-mercaptoethanol (2ME) and DNA drugs, as well as larger bioentities, such as extracellular vesicles and biological cells.

Here, we extend the capabilities of the platform to the attachment-release of wound-healing drugs with different structures and investigate this platform for advanced wound regeneration. We are proposing a novel smart wound healing device, which is expected to combine drug delivery and electrical stimulation in one system, controlled by a clean, simple and efficient electrochemical method (Figure 1). To realise the device, we are utilising an electro-spun nanofiber mat, coated with the PEDOT-based conducting polymer. The parameters of the substrates including porosity and surface area of the electrospun fibre mats are being optimised, as well as the conductivity and electrochemical activity of the substrate upon coating PEDOT. Currently, we are investigating electrochemical attachment - release of various drugs.

Percolation-Controlled Carbon-based Nanomaterials for High Performance Dielectric Composite Materials

Professor Segi Yu[1], Dr. So-Yeon Jun[1]
[1]Department of Physics, Hankuk University of Foreign Studies, Yongin, South Korea

Poster Session, Exhibition Area, February 11, 2025, 12:45 - 13:45

For polymer-based dielectric composite materials, conducting nanomaterials are mixed as a filler to enhance the performance of dielectric materials. Carbon nanotubes (CNTs), as one-dimensional (1D) nanomaterials [1], and graphene, as a two-dimensional (2D) nanomaterial [2,3], are widely utilized. The high dielectric performance, especially, high dielectric constants are easily obtained; but, at the same time, high dielectric losses occurred, which is strong demerit of dielectric composites. It was mostly caused by metal insulator transition (MIT) by addition of conducting nanomaterials. The merits of interfacial polarization due to the existence of conducting nanomaterials were weakened by the demerits of percolative connection among nanomaterials. Thus, to overcome this percolation phenomenon, several methods are devised. For 1D, the length of CNTs were shorted to suppress the percolative connection of CNTs. AC electroluminescence devices, which had a dielectric layer with shortened CNTs, yielding to 50% brighter and 30% less current than the reference devices. In 2D, graphene was used to encapsulate barium titanate particles, to elaborate the interfacial polarization. The encapsulation yielded to 1.5 to 2.2 times higher dielectric constant values than the reference sample. The mild increment of ~20% was obtained in the dielectric loss. This is quite low, when compared with non-encapsulation cases of several times increment. Therefore, we can say that controlling percolation in the conducting nanomaterials is a key factor for high performance dielectric composite materials.

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