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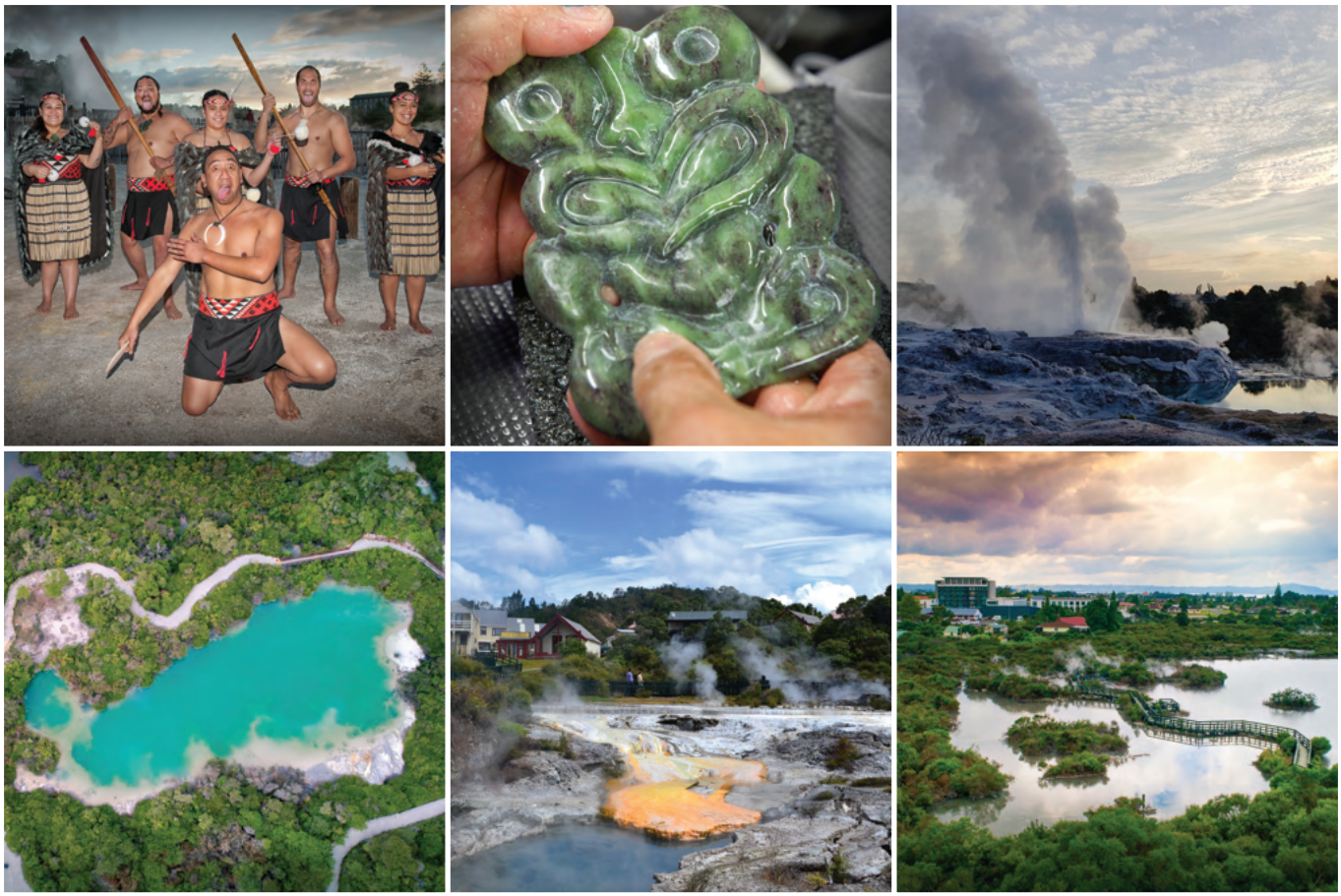

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Oral presentations

Pl.01 Growing a Mātauranga Māori space in the MacDiarmid Institute

Pauline Harris[1]
[1]*Massey University, Palmerston North, New Zealand*

Plenary Session 1, Bay Trust Forum, February 7, 2023, 10:15 AM - 10:45 AM

Māori are the indigenous people of Aotearoa New Zealand. Originating from the Eastern Pacific, they brought with them knowledge and technology that developed and evolved over millenia in areas such as astronomy, navigation, horticulture, medicine and many other sciences. The arrival of Europeans is recent with Abel Tasman being the first to arrive in 1642 and then James Cook arriving in 1769. The history since then has been fraught by colonial injustice which has led to loss of life, land, knowledge and language. This has been exacerbated by urban migration of Māori from their tribal areas to urban towns and cities distancing them from their homelands and knowledge base. Education systems designed to systematically integrate Māori into English language and culture occurred and is still occuring whereby educational institutions still fail to honour the Treaty of Waitangi that underpins our nation. Systematic racism is present throughout including that of the education sector and science sector leading to growing inequities for Māori.

In the last ten years we have seen a significant shift and growth of the nation to engage and embrace Māori culture and language. These shifts have seen the establishment of a Mātauranga Māori based public holiday, Matariki the Māori New Year and the inclusion of Māori history and knowledge into the education system. These shifts have also been seen in the RST&I sector. Where policies such as Vision Mātauranga have had a stronger requirement to be implemented to ensure the inclusion of Māori people, Māori knowledge and Māori language in order to give Māori a place to grow, develop and thrive. Within the context of the Centres of Research Excellences (COREs) such as as the MacDiarmid Institute we are seeing significant increase in the commitment to Māori in some of these COREs. Within the materials and nanotechnology space the MacDiarmid Insititute in this last five years has created a Māori research programme, a deputy director postion and leadership within the science executive. Also one of the highlights has also been the creation of the Discovery Scholarship programme that is aimed to increase the number of Māori and Pacific Island students studying both Māori and Western science. In this talk I will describe and showcase these initiatives and how the MacDiarmid Insititute is contributing to the aims and aspirations of Māori in the science space.

K.01 Science and Mātauranga Māori: Some Thoughts

Charles Royal[1]
[1]*Independent, Auckland, New Zealand*

Keynote Session 1, Bay Trust Forum, February 7, 2023, 11:15 AM - 11:55 AM

Charles Royal will present his views regarding the relationship between science and mātauranga Māori. He will discuss what he regards mātauranga Māori to be and will describe its current 'state'. He will discuss how he believes that the 'seeds' of science, at least, if not a kind of science, exists in mātauranga Māori represented in its pragmatic dimensions. He stresses that this is not a mature science, such as we know today, and argues that it could not be given the history of colonisation and the attacks sustained upon mātauranga Māori. However, he will also assert that because no comprehensive study on the relationship between science and mātauranga Māori conducted by authorities in both knowledge systems has ever been conducted, it is premature to take final positions either for and against.

Charles's motivation concerns equipping tangata whenua communities with high quality knowledge which will enable them to successfully address needs, problems and opportunities of the 21st century. Within this general frame, Charles wishes to build a mātauranga Māori bridge into science by showing how a kind of science already exists within mātauranga Māori and how an indigenous intellectual tradition existed and exists. He wishes to ensure that unfounded assertions about mātauranga Māori are not made and wishes to demonstrate that the major complaints that Māori have with science are not so much with science itself but rather with the machinery and instruments of science which came into Māori communities through the vehicles of colonisation.

K.02 Integration of low dimensional materials for sensing applications

Professor Rebecca Cheung[1]
[1]*University of Edinburgh, Edinburgh, United Kingdom*

Keynote Session 2, Skellerup & WSP, February 7, 2023, 11:15 AM - 11:55 AM

The presentation will describe research conducted on the integration of low dimensional materials for sensing applications. In particular, the design, fabrication and characterization of graphene based membrane resonators for acoustic sensing, ZnO nanowire force sensors and pyroelectric infrared sensing amplified by two-dimensional transistor will be presented.

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K.03 Technology for Bioelectronic Medicine

Professor George Malliaras[1]
[1]*University of Cambridge, Cambridge, UK*

Keynote Session 3, Bay Trust Forum, February 7, 2023, 11:55 AM - 12:35 PM

Bioelectronic medicine provides a new means of addressing disease via the electrical stimulation of tissues: Deep brain stimulation, for example, has shown exceptional promise in the treatment of neurological and neuropsychiatric disorders, while stimulation of peripheral nerves is being explored to treat autoimmune disorders. To bring these technologies to patients at scale, however, significant challenges remain to be addressed. Key among these is our ability to establish stable and efficient interfaces between electronics and the human body. I will show examples of how this can be achieved using new organic electronic materials and devices engineered to communicate with the body and evolve with it.

K.04 The grand design of new class of materials and properties

Professor Xiaolin Wang[1,2]

[1]*Institute for Superconducting and Electronic Materials, University of Wollongong, North Wollongong, Australia,* [2]*Australian Research Council Center of Excellence in Future Low Energy Electronics Technologies, University of Wollongong, Australia, North Wollongong, Australia*

Keynote Session 4, Skellerup & WSP, February 7, 2023, 11:55 AM - 12:35 PM

The discovery of new materials with superior performance will promote the rapid development of science and technology and will change and improve our daily lives. However, discovering new materials and properties is challenging due to their complexity in both materials chemistry and physics. How many of them are still waiting for us to explore and discover? What are they? How do we know or design them? These are the ultimate questions and goals of the grand design of new materials and properties. In this talk, I will summarize the conventional methods used in material design and introduce new strategies for the grand design of new materials and properties. I will highlight how to design new materials and properties based on new electronic states, new band structures, new states of matter etc. I will present some of the novel materials and properties we have designed for both solids and liquids, including new quantum materials with unique charge and spin attributes for novel electronics, spintronics, topological electronics, and dissipationless transport.

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I1A.1 Te Tai Hauāuru O Te Ika Whenua – Convergence of West Coast terrestrial ecosystems from the great fish of Māui

Ms Diane Bradshaw [1]
[1]*Partnerships GNS Science & MacDiarmid Institute*

1A | Science in Society, Bay Trust Forum, February 7, 2023, 1:30 PM - 3:30 PM

Twenty-five million years ago, tectonic plate movement and volcanic activity forged a new set of islands on the edge of a zone of intense seismic activity known as the Ring of Fire. Much of Aotearoa is mountainous a young country where mountains are still rising, where earthquakes occur frequently as the earth's crust yields to pressures deforming Papatūānuku (the land).

Traditions of Maui the explorer describes how the island emerged was formed and is still being shaped by nature's forces of volcano, wind, and water. Earths 8th Continent Zealandia together with cultural traditions informs geological processes that shape Te Riu-a-Māui as well as enriches Māori and Pasifika narratives of exploration and discovery.

Te Riu-a-Māui literally means the hills, valleys and plains of Māui - the great East Polynesian ancestor explorer of the Pacific Ocean. Riu means hull (of a canoe), basin (like the Waikato basin), a belly, the core (of a body) forming stronger connection to and acknowledgement of our natural world.

Waikato regions west coast Kawhia and Aotea harbours are of immense value to Māori and are intimately connected to these traditions associated to tribal whakapapa (genealogy), tikanga (values) to guide whānaungatanga (kinship).

In this talk, I will share Māori philosophical worldviews combined with materials research along our every changing coast-line. Prioritising adaptation planning processes of adjustment to impacts of climate change. Actions that incorporate, customary values and practices linked to Māori wellbeing and sense of identity of both the Tainui and Aotea a waka (canoe) legacy of migration.

I1A.2 Nanoscience Education as a Vehicle to Enhance Scientific Literacy

Dr. Swarna Basu[1]
[1]*Susquehanna University, Selinsgrove, United States*

1A | Science in Society, Bay Trust Forum, February 7, 2023, 1:30 PM - 3:30 PM

Advances in science and technology are often met with questions about safety, equitable access, skepticism, and on occasion, misinformation and pseudoscientific counterarguments. Most recently, the use of lipid nanoparticles in the mRNA Covid-19 vaccines has given rise to several conspiracy theories about the presence of "nanobots" or some form of nanomachine that serve as government tracking devices. Among the many ways to alleviate concerns about scientific advances and the implementation of anything that appears to be new technology is to enhance science education at the K-12 and college levels and improve how science is communicated to the public. Given the interdisciplinary nature of nanoscience, courses and programs in this field can serve as an effective vehicle for improving scientific literacy and communication, while also enhancing the education experience for those in related areas.

Using the development and implementation of a special topics course in nanoscience at an undergraduate institution in the United States as an example, this presentation will highlight how the newest ideas and developments in the field are introduced to students. The course design includes an overview of foundational concepts, discussion of ethical and societal implications, the funding process, effective strategies for the dissemination of news about breakthroughs, and hands-on activities that can also be incorporated into lower-level courses and even the K-12 level. The final aim of this presentation is to show that nanoscience education, and even research, need not be a specialized field limited to investigators at large research institutions and those undertaking post-graduate studies.

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1A.1 Ngā Wai Ariki O Whakarewarewa He Kohikohinga Hau Kāinga – Perspectives, partnerships social-natural hazard materials of geothermal taonga

Miss Ringahora Huata[1,2]
[1]*MacDiarmid Institute of Advanced Materials and Nanotechnology, New Zealand*
[2]Australian Research Council

1A | Science in Society, Bay Trust Forum, February 7, 2023, 1:30 PM – 3:30 PM

The nature of Māori culture and values presents an opportunity to reimagine the scope of community resilience that derive through the generations. The oral history of Māori has seen resilient practices weaved into the very nature of their culture, which knowledge has survived through the oral transmission of songs, proverbs, and stories. Deriving this information from a people so aligned and immersed in nature is the knowledge required to improve and respond to the natural environment while expanding literature to explore and innovative to improve the lives of people in Aotearoa. This information will be compared to modern Māori perceptions of the local Iwi Tuhourangi, Ngāti Wahiao, located in the city of Rotorua. According to the Māori whakatauki/Maori proverb 'he aha te mea nui o te ao? He tangata, he tangata, he tangata or 'what is the most important thing in the world? It is people, people, people'. The concept is based upon the natural world as a divine inheritance as potentially with Māori values relating to land, air, water resource. This paper will enable the expansion of Māori culture that recognises the importance of research partnerships as a platform for intersecting with the theme of sustainability science and society.

1A.2 Knowing and growing a student's strengths profile: How to assess and enhance transferrable skills in a university student

Dr Andrea Kolb[1], Ms Judith Marecek[2], Dr Yantao Song[3]
[1]Faculty of Engineering, The University of Auckland, Auckland, New Zealand, [2]Centre for Innovation and Entrepreneurship, The University of Auckland, Auckland, New Zealand, [3]Technical Services, The University of Auckland, Auckland, New Zealand

1A | Science in Society, Bay Trust Forum, February 7, 2023, 1:30 PM - 3:30 PM

Employers expect university graduates to have an appropriate strengths profile, including discipline-specific competencies and transferrable skills (Khoo et al., 2020). High employability is often associated with the following skills and attributes: creativity, persistence, self-confidence, long-term vision, optimism, and planning and organising (Tymon, 2013). Fostering these transferrable skills in a student improves their self-efficacy, paving their career pathway toward leadership and societal and economic value creation (Rae and Melton, 2017).

This talk discusses a learning framework for assessing and developing transferrable skills in undergraduate Chemical & Materials Engineering students as part of their coursework. The framework is grounded in Constructivism and uses problem-based learning (Savery et al. 1995). The learning objectives help students understand and enhance their transferrable skills scales. Summative, formative, individual and team assessments track the progress of a student's skills enhancement. They include, e.g., psychometric tests and questionnaires, creating a project proposal, writing self-reflections, giving peer feedback, and presenting outputs and outcomes. The coursework and problems posed are centred around a toy-sized hydrogen fuel cell car and using rapid prototyping techniques (e.g., 3D printing and laser cutting), appealing to the passions of engineering students. Addressing students' interests engages them deeply in their coursework and assessments, designed to know and grow their transferrable skills profile.

The framework is intuitive, adjustable, scalable and transferrable, making the techniques and tools discussed valuable and applicable to a wide range of science and engineering educators and programs.

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1A.3 Research mentoring to increase diversity in STEM

Dr. Colleen Marlow[1]
[1]*California Polytechnic State University, San Luis Obispo, San Luis Obispo, United States*

1A | Science in Society, Bay Trust Forum, February 7, 2023, 1:30 PM - 3:30 PM

Undergraduate research is a high-impact practice known to increase engagement and retention of underrepresented populations in STEM (1). An essential element in the success of these experiences for increasing diversity in STEM fields is faculty mentoring (2). How individual faculty mentor their research students has individual and collective impacts on the accessibility, inclusivity, and equity of research experiences and the current and future diversity of STEM (3). Yet, most faculty have not been trained or supported to develop intentionally accessible, inclusive, and equitable mentoring practices (4). Even when faculty desire to improve their mentoring practices by participating in university-wide professional development programs, barriers exist – these include time, workload, variations in prior knowledge, and perceptions that disciplinary differences prevent universal best practices which often lead to trainings that are highly theoretical. For trainings to be worthwhile they must deliver practical solutions ready for implementation while also meaningful engaging faculty in diversity work. I will present a recently developed faculty workgroup model designed to train faculty for more accessible, inclusive, and equitable undergraduate research mentoring. This workgroup was piloted with 5 physics faculty at Cal Poly San Luis Obispo over an 8-week period. In addition to discussing the outcomes of the workgroup, I will provide examples of mentoring resources developed. While this talk focuses on undergraduate research mentoring the content, methods and practical tools presented are relevant and transferable to graduate research mentoring.

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1A.4 Hydrogen: An opportunity to teach thermodynamics

Professor Aaron Marshall[1,2], Mr Garrick Thorn[1]
[1]*University of Canterbury, Christchurch, New Zealand,* [2]*MacDiarmid Institute of Advanced Materials and Nanotechnology, New Zealand*

1A | Science in Society, Bay Trust Forum, February 7, 2023, 1:30 PM – 3:30 PM

Hydrogen is seen by many as a useful energy carrier and chemical feedstock for many industries. But it is not a panacea for climate change or energy security. It is critical to educate the public and next generation of scientists, engineers and policy makers about its pros and cons so that sensible decisions in the future can be made. This talk will focus on various outreach opportunities and how hydrogen can be used as a general example to explain energy transformations, storage, and distribution. We will also discuss the development of a hands-on experiment involving water electrolysis and how this can teach students everything from thermodynamics, process economics and sustainability.

I1B.1 Uncovering electron transfer pathways: towards the rational design of light-harvesting molecules

Dr Georgina Shillito[1], Dr Stephan Kupfer[1], Professor Benjamin Dietzek-Ivanšić[1], Professor Sven Rau[2], Professor Keith Gordon[3]
[1]Friedrich Schiller University Jena, Jena, Germany, [2]University of Ulm, Ulm, Germany, [3]University of Otago, Dunedin, New Zealand

1B | Catalysis 1 – electrocatalysis and nanomaterials, Skellerup, February 7, 2023, 1:30 PM - 3:30 PM

There is an ever-pressing need for clean, renewable energy sources. With sufficient solar energy incident per day on the earth's surface to meet global energy requirements for an entire year[1], utilisation of this resource seems like an obvious choice. However, a significant challenge remains in artificially replicating the light-harvesting processes which nature conducts with ease. Nonetheless, significant progress has been made in the design of molecular photosensitisers for a range of applications, including dye sensitised solar cells and hydrogen generating photocatalysts.[2-3]

In general, molecular photocatalysts require three, usually separate components; a photoactive moiety, an electron relay and a catalytic centre. However, intramolecular systems, where all components are found on the same molecule, are of considerable interest. Recent studies of Ru(II) (photosensitiser) complexes possessing a tetrapyridophenazine bridging ligand (electron relay) and an additional chelated metal (catalytic centre), have been shown to demonstrate photocatalytic activity.[3-5]

Quantum chemical methods, such as density functional theory (DFT) and time-dependent (TD)DFT, in conjunction with spectroscopic techniques, can provide insight into the mechanisms involved in the conversion of sunlight into electrical energy or molecular hydrogen. Experimental and theoretical investigations of different types of photoactive molecules, ranging from small, model systems, to functional photocatalysts are discussed.[3-6] A greater understanding of the photophysics of such systems, allows new investigative pathways for improving the design of light-harvesting molecules to be explored.

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I1B.2 Modelling light absorption in hybrid core-satellite metal nanostructures

Baptiste Auguie[1]
[1]*Victoria University Of Wellington, New Zealand*

1B | Catalysis 1 – electrocatalysis and nanomaterials, Skellerup, February 7, 2023, 1:30 PM - 3:30 PM

Hybrid nanoparticles combining plasmonic and catalytic components, such as Au and Pd, are being developed for applications in photocatalysis [1–3]. The plasmonic element improves the light-harvesting efficiency of the compound nanostructure and channels this energy toward the catalyst surface. Finding an optimum configuration for the two materials is currently an open problem, and the exact mechanisms of energy transfer are also the subject of intense research activity [1,4].

We have studied several Au–Pd based nanostructures, in the form of core-shell and core-satellite assemblies, and tested their photocatalytic activity for H2 generation under simulated sunlight conditions. I will present two electromagnetic models used to simulate light absorption within such nanostructures: i) rigorous, but time-consuming electromagnetic simulations using the superposition T-matrix method [5]; ii) an original effective-medium model describing the satellites as an anisotropic shell [6,7]. These simulations allow us to estimate the spatial distribution of absorption, which in turn correlates with the generation of hot carriers within the catalyst regions.

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1B.1 Phase Transition and Electrocatalytic Performance of Dichalcogenides of Transitions Metal Alloys

Professor Hong Seok Kang[1]
[1]*Jeonju University, Chonju, South Korea*

1B | Catalysis 1 – electrocatalysis and nanomaterials, Skellerup, February 7, 2023, 1:30 PM - 3:30 PM

In collaboration with experimental works for solvothermal syntheses, crystal structure, and electrocatalytic performance, alloys of transition metal dichalcogenides (TDMCs) have been extensively investigated in the whole composition range. Typical examples are Mo1−xNbxSe2, Mo1−xVxSe2, and Nb1-xVxSe2. In order to understand various experimental results, detailed chemical structures of the alloys have been predicted at different x values based on extensive DFT calculations complemented by configurational entropy. First, all the alloys display Se vacancies of less than 10% depending upon the synthetic temperature. Additional Nb/V vacancies and adatoms can be formed in Mo1−xNbxSe2 and Mo1−xVxSe2. These results are in agreement with our calculation on the alloy formation energy. It shows that the formation of those two alloys are unfavorable, while Nb1-xVxSe2 alloy can be formed quite favorably. Second, Mo1−xVxSe2 and Nb1-xVxSe2 exhibits 2H□1T phase transition at x = 0.7 and 0.3, respectively. The higher stability of the 2H phase in the former alloy can be ascribed to one extra d-electron in a Mo atom with respect to a Nb atom. Third, Nb1-xVxSe2 shows polytypic phases before phase transition, which may have something to do with the best alloy formation tendency in the whole composition range. Finally, Gibbs free energy calculation along the reaction path shows that the best performance for the hydrogen evolution reaction (HER) is due to the defective catalytic surface with Se and/or metal vacancies rather than edge sites, rendering the alloys promising for the HER catalysis.

1B.2 Vibrational analysis of host-guest interactions in porous materials as revealed by synchrotron infrared and DFT studies.

Dr Courtney Ennis[1]
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1B | Catalysis 1 – electrocatalysis and nanomaterials, Skellerup, February 7, 2023, 1:30 PM - 3:30 PM

The spectroscopic analysis of materials using far-infrared light is accessible by the use of synchrotron sources possessing a brightness advantage at these wavelengths. In this region, both chemical and physical properties of a porous material can be interrogated by way of low frequency (large amplitude) torsional and lattice vibrations. The absorption bands of such modes can be informative of morphology, pore and channel topology, as well as sorption phenomena associated with gas and solvent guest species.

In this talk we present work from our recent visits to the Australian Synchrotron THz and Far-IR Beamline, where we have examined a series of porous and thermosalient materials under variable temperature conditions using the beamline ATR stage. These laboratory investigations are accompanied by periodic density functional theory on the crystalline solids, where high symmetry can be exploited to model the entire unit cell performing all-electron geometry and frequency calculations. After evaluating the network environment, host-guest interactions are modeled by relaxing symmetry constraints before vibrational spectra is simulated. Here, measured changes in observed band position and profiles can be rationalised at the molecular level from this coupled theory and experimental approach.

Our group has applied this methodology to reveal (i) host-guest interactions within prototype microporous metal-organic framework(MOF) materials[1], (ii) channel topography in novel isoreticular hydrogen-bonded organic frameworks(HOFs) formed via charge-assisted bonding[2,3], and (iii) the dynamics of thermosalient "jumping crystals" that undergo phase transition via specific vibrational "gateway" modes[4]. Insight toward how these phenomena have been elucidated by pDFT modelling will be highlighted.

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1B.3 Something about bubbles - a novel system design for testing catalysts for PEM/AEM electrolysis in an approximated MEA stack

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In developing new catalysts for water splitting reactions, it is important to measure the catalysts in a way that reflects the materials true behaviour in a real-life system. As proton- and anion-exchange membrane water electrolyser (PEMWE and AEMWE) technologies gain in interest and industry traction, it is not sufficient to demonstrate the electrochemical properties in idealised conditions, such as three electrodes or rotating disc electrode experiments.[1] These set-ups do not replicate the complex transport mechanisms in membrane electrode assembly (MEA) stacks and the results of such experiments may not accurately reflect the catalyst activity that will be achieved in a full electrolyser system.[2, 3] Working with catalysts on ion exchange membranes is also tedious as membranes are prone to swelling/warping and it is difficult to achieve low contact resistance.[4-6]

In this work we present a new system for testing novel catalyst materials in an electrochemical system, more closely replicating the conditions of a MEA stack to give more accurate information about the performance of the catalyst in-situ. This system is composed of a sample holder that can replicate a full or half stack MEA with electrolyte flow to better emulate the mass transport parameters of an electrolyser. This system has been used to characterise catalyst coated membranes and standards that have also been characterised in an electrolyser and three electrode set up to verify measurements from the new system, showing increased accuracy when predicting the performance of catalyst materials of a PEM stack compared to the traditional three electrodes system.

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1B.4 Development of Non-Noble Metal Based Catalysts For Hydrogen Production By Seawater Electrolysis

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The increasing energy demand and rapid fossil fuel consumption have triggered the need for alternative energy sources. Hydrogen is the most desirable clean energy carrier owing to its huge gravimetric energy density. For producing hydrogen, water electrolysis is a highly sustainable, zero-carbon technique. However, current technology involves using fresh water, which strains the water resources. The utilization of seawater, which is an abundant source (96.5% of the earth's water), can alleviate this problem. However, its use is hindered by the undesirable chlorine evolution reaction (CER) at the anode and its corrosive effects. Current electrocatalysts are based on scarce noble metals, which increase the cost. This necessitates the development of non-precious metal-based efficient hydrogen evolution reaction (HER) catalysts and highly selective oxygen evolution reaction (OER) catalysts.

In the present work, an assembly of a zeolitic imidazolate framework (ZIF67) derived cobalt-cobalt oxide-carbon composite based anode and nickel-carbon composite based cathode is explored for hydrogen production from alkaline seawater. In contrast to the usual metallic foam substrates, a carbon substrate is utilized here owing to its conductive network and anti-corrosive nature. The highly porous nature, nitrogen-doped hollow structure, and the vast number of active metal sites of the ZIF67-derived material enhances its OER selectivity over CER. The ZIF67-derived material anode and nickel-carbon cathode assembly exhibits a seawater splitting potential of 1.8 V at the benchmark current density of 10 mA/cm2 with a stability over 24 h. Further, a single cell with the membrane electrode assembly (MEA) is fabricated, and hydrogen evolution is demonstrated.

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I1C.1 Remarkable nano-patterning in liquid metals

Dr. Krista Grace Steenbergen[1], Prof. Nicola Gaston[2], Dr. Stephanie Lambie[2], Dr. Charlie Ruffman[2]
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20 second overview

Fascinating patterns – including spots, zebra stripes, wiggles and cubes – emerge from doped liquid metal systems. Using first-principles (DFT) simulations, we explore the physical and chemical origins of this nano-patterned self-assembly.

More detail

A pool of liquid metal … a pattern slowly emerges from beneath the opaque surface. It reads like science fiction, but nano-patterns self-assembling on the surface of liquid metals has recently become a science reality. Experimentalists at UNSW can now create an intriguing range of patterns and shapes – stripes, spots, rods, cubes, even complex Turing patterns (Fig. 1) – by solidifying liquid metals mixed with different dopants. Recently, experimentalists demonstrated that a gallium liquid doped with platinum tripled catalytic activity (compared to the solid system).¹ Other liquid metal systems show enormous promise for advancing a wide range of technological fields, including optics, electronics, sensing, and renewables.

Using first-principles (DFT) simulations, we investigate the origins of nano-patterning, including the physical and chemical properties that guide the diffusion and self-assembly of the dopants. I will present an overview of our recent results (experimental and theoretical) on liquid gallium doped with a diverse range of elements.²⁻⁵ I will also discuss future directions and a few of the interesting technologies emerging (literally) from this research.

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I1C.2 Surface-Grown Crystalline Patterns and Structures from Liquid Metal Solvents

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1C | Liquid metals, WSP, February 7, 2023, 1:30 PM – 3:30 PM

The liquid-to-solid transition of a supercooled liquid alloy creates separated crystalline phases. Mediated by phase transition energetics and structural characteristics, these emergent phases self-organise into well-defined solidification patterns and structures. In the presence of a strongly interacting metallic solvent, the unique phase interactions and growth dynamics can lead to novel phase transition and crystal growth pathways. In addition, when crystal growth takes place at a liquid metal's surface, asymmetric growth conditions and surface effects arise; and as a result, crystals with morphologies distinct to their bulk solidification counterparts can form.

In this talk, our recent works [Ref 1&2] on the solidification patterns and structures grown in dilute alloy systems will be presented. The characteristic features, including ordering and phase enrichment, of the surface solidification effect and the surface emerged patterns will be demonstrated. Taking advantage of the surface/interfacial nature, possible strategies utilising the surface solidification platform for studying fundamental phase transition and crystallisation processes, and for controlling surface crystals will be proposed. I will then conclude with remarks on future works and applications.

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1C.1 Liquid metal-based synthesis of functional 2D materials for electronic applications

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1C | Liquid metals, WSP, February 7, 2023, 1:30 PM - 3:30 PM

Many metals feature an atomically-thin oxide layer at the metal air interface.[1] A classic example is aluminium which is stabilised in air by its surface oxide. This also applies to low temperature liquid metals including molten tin, indium, gallium and their alloys. This oxide layer typically grows in a self-limiting reaction, providing a synthetic pathway towards ultra-thin, two-dimensional materials.[2] In recent years, several liquid metal-based synthesis strategies have been developed that allow isolating these naturally occurring 2D materials, resulting in laterally large nanosheets with highly reproducible thickness. These oxides can then be directly used or processed further into desired compounds.

Interestingly, liquid metal-based synthesis strategies allow isolating nanometre-thin nanosheets of non-stratified materials, providing an opportunity to drastically increase the number of accessible 2D materials.[2]

This talk will provide an introduction into liquid metal chemistry and will demonstrate how large area ultrathin nanosheets can be isolated form the liquid metal interface. The synthesized materials are ideally suited for a variety of applications including electronics, piezotronics and catalysis.[4-8]

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1C.2 Atomistic control for self-assembly of nanostructure

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1C | Liquid metals, WSP, February 7, 2023, 1:30 PM - 3:30 PM

The manipulation of interatomic interactions for structural self-assembly is a seductive promise of nanotechnology, most tantalisingly made evident by biological examples in nature. Much of the promise of sustainability in materials science comes from the idea of such structural control, at low energetic cost. At the risk of anthropomorphising atoms, this talk will present some examples of how, by developing an understanding of how particular atoms want to behave, we can manipulate structure by proxy. Not through forcible manipulation of atoms, but through understanding their environmental preferences, and how these change through many-body interactions as they assemble.

The control of nanostructure through understanding electronic shell structure will be used as one example, with reference to metallic clusters known as superatoms [1]. In this case, electronic interactions and symmetry rules provide clear predictive rules for the development of nanostructure, and indeed, for the emergence of electronic structure in nanostructured assemblies.

On the other hand, recent work looking at interactions in dilute metal alloys [2] has provided evidence of structural control at liquid-solid interfaces. The use of ab initio methods will be outlined for these two cases, and the challenges of dealing with complex nanostructures and finite temperature simulations discussed.

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1C.3 Two-dimensional (2D) p-type semiconducting oxide from liquid metal alloy

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Two-dimensional (2D) materials have attracted significant interests from the research and industrial communities due to their unique physical and chemical properties. Although various synthesis approaches exist, some possess complex optimisation and require high operating temperature, which precludes synthesis of some materials. Liquid metals (LMs) and metal alloys offer an alternative 2D material synthesis platform as the Cabrera-Mott oxidation reaction occurs at the solid-gas interface once exposed to ambient conditions.1 As a result, a smooth and ultrathin oxide layer attaching weakly to the LM solvent forms, which can then be transferred onto desired substrates. To date, several LM-based syntheses have been developed and gained popularity since they offer scalable, low-temperature, cost-effective, and vacuum-free alternatives to the conventional processes. Furthermore, naturally non-stratified materials can be obtained thanks to these techniques. In this work,2 we presented a roll-printing method performed on liquid eutectic chalcogen mixture (selenium-tellurium) to synthesise a novel 2D tellurium oxide (β-TeO2). Theoretically, this material owns promising properties for electronic applications and has never been experimentally explored. The isolated 2D oxide was subsequently integrated into a basic electronic device and exhibited remarkable performances paving a way to a development of advanced applications.

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1C.4 Liquid metal derived atomically thin indium nitride (InN) films featuring 2D electron gases

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1C | Liquid metals, WSP, February 7, 2023, 1:30 PM - 3:30 PM

Indium nitride (InN) is a promising semiconductor for optoelectronics [1] since it possesses a narrow bandgap [1], high carrier mobilities [2], and also intriguing characteristics of accumulating free electrons along its surface region [3]. However, the realization of 2D InN remains intangible due to the synthesis complexities associated with its low dissociation temperature and high equilibrium vapor pressure of nitrogen [4]. Herein, we report the synthesis of ultra-thin InN and tin-doped InN (Sn:InN) with lateral dimensions exceeding centimeter-scale, suggesting that incorporation into classic wafer-based technologies may be achieved with ease. The synthesis is carried out via a two-step liquid metal-based printing method [5] followed by a micro-wave plasma-enhanced nitridation reaction. Ultra-thin InN nanosheets with a thickness of ~2±0.2 nm were isolated over large areas with lateral dimensions exceeding the centimeter scale. Room temperature Hall effect measurements reveal carrier mobilities of ~216 cm2 V-1 s-1 and ~148 cm2 V-1 s-1 for undoped and doped InN, respectively. We demonstrate that the incorporation of Sn dopants leads to a significant enhancement of the intrinsic plasmonic properties of InN due to an increased carrier density. Moreover, the presence of discrete and quantized states at the surface of InN was observed and comprehensively investigated. Density functional theory-based analysis of ultra-thin InN reveals the presence of interfacial electron accumulation layers forming a 2D electron gas in the as-synthesized nitride nanosheets. Overall, the combination of electronic and plasmonic features in undoped and doped ultra-thin 2D InN holds promise for creating advanced optoelectronic devices and functional 2D heterostructures.

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I1D.1 Two-dimensional materials for next-generation electronics and optoelectronics technologies

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1D | Optical materials 1, Downer, February 7, 2023, 1:30 PM - 3:30 PM

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 light operated artificial- synaptic and logic devices and neural networks that can recognise numbers and patterns. 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 a range of industry partners.

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I1D.2 III-V Quantum Dots, Seeing Light and Dark

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1D | Optical materials 1, Downer, February 7, 2023, 1:30 PM - 3:30 PM

III-V quantum dots are printable semiconductors free of hazardous substances. In this talk, recent progress in III-V QD synthesis at Ghent University and the device implementation of these materials is discussed. First, we show that the formation of InP-based QDs with near-unity photoluminescence quantum yield across the visible spectrum is now possible, and discuss the properties of monochromatic LEDs made using such QDs as on-chip color convertors. Second, we demonstrate the synthesis of In(As,P) QDs with a band-edge absorption up to 1600 nm, and demonstrate the formation of QD photodiodes sensitive up to 1400 nm from these QDs. Both examples highlight how III-V QDs are evolving from a material for lab-scale proof-of-principle to devices ready of the cojianbonsumer-market

1D.1 Hybrid organic/inorganic nanomaterials - A new type of optoelectronic material.

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Recently, there has been an increase in research into the field of organic semiconductor ligands attached to nanocrystal semiconductor quantum dots, essentially the replacement of ligands that offer colloidal stability with ones that add additional optoelectronic properties. By combining the ease of attachment/functionalisation of the organic component with the tunability (via confinement effects of QDs, hybrid nanomaterials present a new and versatile class of optoelectronic materials with properties beyond the sum of the individual components. We use this versatility to make improvements across different optoelectronic disciplines such as luminescent solar concentrators, spectral management systems (up and down conversion), photocatalysis and lasers.

1D.2 Whispering Gallery Mode Lasing from Perovskite Nanocrystals Chemically Attached to Microcavities

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All inorganic lead halide perovskite based microlasers have received much attention since they were shown to have low amplified spontaneous emission thresholds in 2014(1). Many different lasing arrangements have been made all with different focuses, such as ultra-low lasing thresholds, ultra-high Q factors, unidirectional output, or high stability(2–5). My research is focused on achieving ultra-low thresholds and high Q factors with a previously used lasing set-up focused on high thermal- and photo-stability. This was CsPbBr3 nanocrystals chemically attached to silica microspheres for whispering gallery mode lasing(5). So far, the first focus of my research has been on increasing the consistency and yield of the synthesis. This has involved optimizing the conditions of the synthesis in various ways and trying new methods as well. I have also begun investigating how the size of the spheres and type of spheres (e.g. hollow or solid) affect the observed lasing characteristics.

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1D.3 Gallium Phosphide nanostructures as versatile platform for nonlinear and ultrafast nanophotonics

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Gallium phosphide (GaP) is a well-known semiconductor with a high refractive index (around 3.3 in the visible) and a large optical bandgap of 2.2 eV, making it transparent for a large part of the visible spectrum. Furthermore, amorphous and crystalline thin films can be fabricated on transparent substrates, making GaP an excellent candidate for nanophotonic applications.

In our work, we thoroughly characterize GaP thin films with respect to their linear and nonlinear optical performance. We show that crystalline thin films reach an absolute second-harmonic generation (SHG) efficiency that is comparable to the bulk crystal and determine its second-order nonlinear susceptibility to be one order of magnitude higher than for common nonlinear crystals. The amorphous film on the other hand, lacking a second-order nonlinear signal, outperforms crystalline GaP third-harmonic generation (THG) absolute efficiency. Furthermore, we show that by nanostructuring the films and performing optical excitation around the anapole resonance, efficient SHG[1] and record value all-optical switching can be achieved, reaching a modulation depth of 20 % and possible modulation speeds up to 20 THz[2]. Finally, we investigate hybrid nanostructures consisting of GaP, incorporating a 20 nm thin layer of indium tin-oxide (ITO) in the center. By excitation around the epsilon near-zero wavelength of ITO, we investigate the coupling of the two materials and the strongly enhanced nonlinear response.

In conclusion, we emphasize the excellent optical properties of GaP and in particular its possible applications for nonlinear nanophotonics.

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1D.4 Single-mode THz vibronic coherence contributes to suppression of nonradiative rates in molecular aggregates

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1D | Optical materials 1, Downer, February 7, 2023, 1:30 PM - 3:30 PM

Vibronic coherences (VC) in solid state have gained broad spectrum of interest for their potential roles in influencing photophysical and photochemical processes, and the underlying mechanism facilitates energy-conversion applications such as photocatalysis, photovoltaics and luminescent materials. Realizing the significance for the VC-based device developments, we have investigated the advantages of VC in molecular solid that reveals new material properties. In this study, we focus on the ultrafast dynamics of the self-assembled Pt(II) complex 4H, its derivatives and other NIR emissive Pt(II) complexes in a solid film, which have been reported to exhibit high intense near infrared (NIR) emission and hence high performance organic light emitting diodes (OLEDs) in our previous reports [Nat. Photonics 2017, 11 (1), 63–68, Nat. Photonics 2020, 14, 570-577 and Nat. Photonics 2022, accepted]. We utilized the transient absorption spectroscopy (TAS) driven by a ytterbium-based multiple-plate compression (MPC) light source, which provides ultrafine and adjustable time resolution up to as fast as 3.2 fs. Based on MPC-TAS, a single-mode VC of 32 cm-1 (0.96 THz) was observed in the 4H solid film, which retains during ultrafast intersystem crossing with a lifetime of 150 fs. To elaborate the high NIR emission efficiency of the self-assembled Pt(II) complexes, we prove that the conservation of single-mode VC contributes to the suppression of nonradiative rates via reducing the vibronic frequencies associated with excited-state deactivation. The results infer that well-aligned molecular solid with significant intermolecular charge-transfer optical transitions are promising candidates for luminescent materials. This study provides a novel perspective of VC, which stimulates further investigations on correlation among vibronic coherence, exciton delocalization and exciton-vibration coupling in molecular solids and their effects on device performances.

I1E.1 A Subdural Bioelectronic Implant for use following Spinal Cord Injury in Rats

A/Prof Darren Svirskis[1], Dr Bruce Harland[1], Dr Brad Raos[1], Brittany Hazelgrove[1], Lukas Matter[2], Dr Simon O'Carroll[1], Prof Maria Asplund[2]
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1E | Bio 1 – Devices and materials, Sigma, February 7, 2023, 1:30 PM – 3:30 PM

Bioelectronic devices have found use at the interface with neural tissue to investigate and treat nervous system disorders. We have developed and characterized a very thin flexible polyimide-based bioelectronic implant that is inserted along the thoracic spinal cord in rats directly in contact with the dorsal surface of the spinal cord. There was no negative impact on hind-limb functionality nor any change in the volume or shape of the spinal cord. The bioelectronic implant was maintained in rats for a period of 3 months. We have obtained the first subdural recordings of spinal cord activity in freely moving animals. Recordings contained multiple distinct voltage waveforms spatially localized to individual electrodes. A clinically relevant spinal contusion injury can be achieved with the implant in place. This device has great potential to monitor electrical signaling in the spinal cord after an injury, and in the future, this implant will facilitate the identification of biomarkers in spinal cord injury and recovery. We are exploring further development of this implant to deliver localized treatments to the spinal cord towards regeneration of damaged tissues to recover lost function. Localized therapies are being developed in the form of pharmaceutical treatment through the local delivery of neurotrophic factors, and electroceutical treatment through precise electrical field stimulation.

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https://onlinelibrary.wiley.com/doi/full/10.1002/advs.202105913

I1E.2 Development progress towards a diamond and carbon fibre brain implant for epilepsy management

Associate Professor David Garrett[1]
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1E | Bio 1 – Devices and materials, Sigma, February 7, 2023, 1:30 PM - 3:30 PM

From the pacemaker to the cochlear implant, the field of neuromodulation implants is making inroads into treating some of medicines most intractable conditions. Drug resistant epilepsy is just such a condition. For the 30% of people who live with epilepsy and do not respond to medication, there are currently no interventions barring resection of brain tissue.

Recent work has shown that seizures can be forecast and potentially avoided following a neuromodulation device implant into the brain. Quality of brain recording is likely to be closely linked to seizure prediction accuracy but current implantable recording technologies are severely limited in both spatial and temporal resolution. For the past ten years, we have investigated novel material combinations with the potential to overcome these resolution limitations. Using integrated diamond and carbon fibre electrode arrays, we are currently demonstrating single neuron, biostable recording, from brain.

This talk will describe the development and diversification of our carbon fibre array technology and describe our progress towards commercialisation of an integrated epilepsy management system.

1E.1 Sustainable Solution for Gut Microbiota Sampling

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1E | Bio 1 – Devices and materials, Sigma, February 7, 2023, 1:30 PM - 3:30 PM

Human gut microbiota (microorganisms) can provide comprehensive information about the health of a host and can act as a biomarker to assist in the early diagnosis of diseases such as cancer, diabetes and obesity [1]-[3]. Furthermore, microbiota helps study human nutrition [3] and can be used to address mental health issues e.g., stress and anxiety [4]. However, the tools to obtain a microbial sample, directly from the small intestine, without contamination are not available [2], [5].

Therefore, in this work, a reusable pill-sized device (robotic capsule) is developed which travels through the gastrointestinal tract and collects samples from different sites of interest and avoids contamination. All the parts of the robotic capsule are reusable and environment friendly. Mainly, a reusable novel actuator (shape memory alloy spring) is designed in this work, which performs opening and closing movements. A specially designed button cell battery (eco-friendly) is used to pass the current through the SMA spring, which changes spring's shape due to induction heating. The developed actuator occupies a small space (5 × Ø4 mm) and produces enough output force (1 N) to function inside the gut. The proposed micro capsule is reusable as compared to commercial endoscopic capsules that cost over $1,000 and are for one-off use only. The robotic capsule prototype, developed in this work, has a potential to become a vital apparatus for clinicians and scientists to sample human and animal gut in the future.

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1E.2 Stiffness-patterned and hierarchical GelMA hydrogels towards in vitro cardiac scar tissue models

Dr Anaïs Chalard[1,2], Harrison Porritt[1,2], Dr Alexander Dixon[3,4], Prof Andrew Taberner[3,4], Dr Annika Winbo[5,6,7], A/Prof Johanna Montgomery[5,6], Dr Juliette Fitremann[8], A/Prof Jenny Malmström[1,2]

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1E | Bio 1 – Devices and materials, Sigma, February 7, 2023, 1:30 PM - 3:30 PM

Scar or fibrotic tissue is generally characterised by an increase in the mechanical properties of the extracellular matrix (ECM) due to the abnormal deposition of proteins such as collagen or fibronectin.[1] To mimic the mechanical properties of healthy and fibrotic tissue in vitro, we use gelatine methacryloyl (GelMA) hydrogels. This biomaterial is inherently biocompatible and allows the precise control of its mechanical properties by controlling the curing process.[2] This latter is done by exposing the pre-gel to visible light for a specific time at a specific intensity. The gels' mechanical properties patterning is achieved via a projection device to create scaffolds presenting both healthy and fibrotic conditions.[3] Our results show that the projection device allows the production of GelMA gels with specific shapes and that patterning the intensity of the projected light results in patterns of elastic modulus such as gradients. We also demonstrate the biocompatibility of the scaffolds by directly encapsulating human induced pluripotent stem cell-derived cardiomyocytes directly into the gels. Finally, to produce hierarchical scaffolds with a more accurate structure closer to natural ECM, we incorporate supramolecular fibres formed by a low molecular weight gelator into the GelMA.[4] These fibres are expected to degrade over time while offering cell guidance in the meantime. Overall, this work offers potential solutions to study cellular behaviours at the interface between healthy and fibrotic tissues.

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1E.3 Deep Eutectic Solvents as Cryoprotective Agentsfor Mammalian Cells

Dr Saffron Bryant[1], Dr Aaron Elbourne[1], Dr Jitraporn Vongsvivut[2], Dr Stephen Holt[2], Dr Tamar Greaves[1], Dr Gary Bryant[1]
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1E | Bio 1 – Devices and materials, Sigma, February 7, 2023, 1:30 PM - 3:30 PM

Cryopreservation has had huge benefits for the world at large, including preservation of blood and stem cells, and assisted reproductive technologies.(1) However, many cell types cannot be stored using current methods, and no organs.(2-4) In fact, 60% of all donated hearts and lungs are discarded due to inadequate storage methods.(5) This waste could be overcome with cryopreservation.

The main limitation in cryopreservation is the ongoing reliance on predominantly just two cryoprotective agents (CPAs), both of which are toxic: dimethylsulfoxide (DMSO) and glycerol.(6, 7) They are also ineffective for many cell types. Thus there is a need for different, non-toxic CPAs with tuneable properties.(8)

Deep eutectic solvents (DESs) are highly tuneable solvents, many of which are non-toxic and have promising properties for cryopreservation.(9) We have characterised a number of DESs for their thermal properties and interactions with mammalian cells, including toxicity and permeability, as well as fundamental studies on membrane and biomolecular interactions. One DES was then carried forward and tested for its cryoprotective effect on four distinct mammalian cell lines. It was just as effective, and in some cases more effective, than DMSO at protecting the cells during cryopreservation.

These results provide new avenues of cryopreservation for cell types which cannot be preserved with existing CPAs. This in turn has wide-ranging benefits, especially in the biomedical field.

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1E.4 Temporal analysis of human mesenchymal stem cells under electrical stimulation with AFM

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1E | Bio 1 – Devices and materials, Sigma, February 7, 2023, 1:30 PM - 3:30 PM

Human mesenchymal stem cells (hMSCs) have great potential for tissue engineering because of promising benefits, sourcing from adult tissue and having multipotent differentiation ability. While external physical stimulation of hMSCs can regulate its fate, it's unclear how these signals induce biological changes. For example, electrical stimulation can induce stem cell differentiation without exogenous growth factors or creating new biomaterials for cells to grow onto.[1]

Cells feel and react to external physical clues via mechanotrasduction to control their own behaviour, including proliferation and differentiation.[2] During the process, cells translate physical signals to biochemical and biological signals and transport into intracellular organelle via cytoskeleton, inducing the mechanical properties change of cytoskeleton, which is crucial to stem cell fate. Providing suitable physical signals and precisely monitoring how cell mechanics change would help elucidate the mechanisms driving stem cell fate.[3]

Atomic Force Microscopy (AFM), a unique technical for non-destructive measurement, is used to characterise cell structure and mechanics. Using Quantitative Imaging mode,[4] we monitored live hMSC in real time, quantifying spatial mechanical properties with high-resolution images, from which we identified intracellular features such as the actin cytoskeleton and peri-nuclear region. An electrical stimulation device was used to apply external stimulation on cells (inducing osteogenesis), while simultaneously scanning with AFM. Combined with the precise measurement of AFM, cytoskeletal changes triggered by external stimulation on stem cells differentiation can be understood. An extraordinary platform has been designed to precisely manipulate cell fate with understanding the effect of external stimulation on cell linage via advanced AFM.

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K.05 New Applications of 2D Materials from Wearable Health to Memory Devices and 6G Switches

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Keynote Session 5, Bay Trust Forum, February 7, 2023, 4:00 PM - 4:40 PM

This keynote talk will present our latest research adventures on two-dimensional (2D) nanomaterials towards greater scientific understanding and advanced engineering applications. In particular, the talk will highlight our work on flexible electronics, zero-power devices, single-atom monolayer memory, non-volatile RF/5G/6G switches, and wearable tattoo sensors for mobile health. Non-volatile memory devices based on 2D materials are an application of defects and is a rapidly advancing field with rich physics that can be attributed to metal adsorption into vacancies. The memory devices can be used for neuromorphic computing and operate as switches up to 500GHz. Likewise, from a practical point, electronic tattoos based on graphene have ushered a new material platform that has highly desirable practical attributes including optical transparency, mechanical imperceptibility, and is the thinnest conductive electrode sensor that can be integrated on skin for physiological measurements including blood pressure monitoring with Class A performance. Much of these research achievements have been published in leading journals.

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K.06 Characterisation of 3D cell cultures systems - challenges and opportunities

Prof Sally McArthur[1], Emma Gill, Miriam Kael, Sorel De Leon, Prof Paul Stoddart
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Keynote Session 6, Skellerup & WSP, February 7, 2023, 4:00 PM - 4:40 PM

Research over the last 5-10 years has shown that cell behaviour in 2D varies significantly from that in 3D, with variations in a range of properties including cell shape, gene profile and migration behaviour. There is increasing demand for reproducible and predictable 3D in vitro models that effectively replicate the tissue of interest and will enable the evaluation of biomaterials and smaller implantable devices. A key goal of then becomes to develop the methods to characterise these systems effectively and ensure that the imaging and assays techniques we typically apply to analysing cell culture can be integrated into these more complex systems. Critically we want to be able to move forward and interrogate these systems in real time. This talk will explore the development and challenges associated with characterising all aspects of 3D cell cultures systems and the opportunities for imaging, nanotechnology, and bioengineering to come together to address the issues

Pl.02 Dynamic Hydrogel Matrices to Study Biology in the 4th Dimension

Dr. Kristi Anseth[1]
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Plenary Session 2, Bay Trust Forum, February 7, 2023, 4:45 PM - 5:35 PM

Our group is interested in the development of macromolecular monomers that can be reacted into crosslinked polymer networks in the presence of living cells and tissues. From a fundamental perspective, we seek to decipher the critical extracellular matrix (ECM) signals that are relevant for tissue development, regeneration, and disease and then design polymeric materials that integrate these signals [1]. From an applied perspective, we use this knowledge to design materials that can promote tissue regeneration and wound healing in vivo. This talk will illustrate our recent efforts towards the synthesis of hydrogel networks for 4D cell culture and regenerative medicine, and how one can dynamically control biochemical and biophysical properties through orthogonal, photochemical click reaction mechanisms. Some specific examples will include the design of hydrogels that promote musculoskeletal tissue regeneration [2], super-swelling matrices to visualize cell-matrix interactions with unprecedented resolution [3], and materials-directed growth of organoids from single stem cells [4]. These efforts will then be placed in the context of designing precision biomaterials to address demands for patient specific products and treatments [5].

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K.07 Carbon Nanotube Field Effect Transistor Platforms for Sensitive and Real-time Sensing

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Keynote Session 7, Bay Trust Forum, February 8, 2023, 8:30 AM – 9:10 AM

Functionalised carbon nanotube and graphene field effect transistors (CNTFETs and GFETs) have been used as the active channel in biosensors, with the future promise of lab-on-a-chip diagnostics strongly motivating the research [1]. The ability to effectively sense analytes depends on multiple factors, the conductivity of the platform [2], the robustness of the functionalisation and the selectivity and function of the receptor [3]. Here we present our recent work on the development of the CNTFET and GFET platforms with aptamers and insect odorant receptors and the different challenges and device constraints we have encountered. We will discuss how the sensitivity of the CNTFETs can be optimised, how functionalisation affects the device performance and the potential for biosensors.

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K.08 Design of Novel Nonbenzenoid π-Electron Systems toward Unusual Yet Stable Functional Materials

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Keynote Session 8, Skellerup & WSP, February 8, 2023, 8:30 AM - 9:10 AM

Aromatic hydrocarbons and their heteroaromatic analogues are playing a dominant role in today's organic optoelectronic materials. On the other hand, nonbenzenoid hydrocarbons and relevant cross-conjugated π-electron systems exhibit attractive properties such as long-wavelength absorption and multistep redox properties, most of which are difficult to achieve with the benzenenoid π-electron systems of similar molecular sizes. However, the difficulties in their synthesis, high reactivity, and lack of appropriate molecular design guidelines pose substantial obstacles to the utilization of these classes of compounds as basic frameworks for superior optoelectronic materials.

To address the above-mentioned issues, we have been focusing on the molecular design based on the annulation of weakly aromatic (hetero)arenes on the nonbenzenoid hydrocarbons in a ring-fused manner. Based on this strategy, we have so far succeeded in synthesizing stable yet unusual π-conjugated systems including dehydroannulenes,[1] nonaromatic[2] or antiaromatic nonalternant hydrocarbons,[3] and pentafulvalene,[4] and unveiled their unusual properties. Alternatively, we also demonstrated that the partial replacement of endocyclic C=C bonds with the isoelectronic thioester moieties is also a powerful approach for attaining a stable cross-conjugated π-electron system isoelectronic with pentafulvalene.[5] We also focus on exploring a new concept in the molecular design of organic functional materials based on nonbenzenoid hydrocarbons.[6] In this presentation, I will describe the overview and some of our recent studies based on this strategy.

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K.09 Low melting point liquid metals based on post transition metals

Professor Kourosh Kalantar-Zadeh[1]
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Keynote Session 9, Bay Trust Forum, February 8, 2023, 9:10 AM - 9:50 AM

Low melting point post transition metals and their alloys establish a group of materials that are now commonly recognised as liquid metals. Liquid metals (LM) offer both liquid state and metallic characteristics and as such present unprecedented opportunities for creating functional materials and devices. In essences, LMs are electronic liquid with enigmatic interfacial chemistry and physics. The properties of LMs including softness that allow free elemental displacements, abundance of freely moving electrons, and their unique interfacial chemistry. The specific physicochemical features of LMs make them promising materials for driving interesting liquid state physics and exceptional chemical reactions on their surfaces for designing nanoarchitectonic systems and also their bulk for developing a variety of systems, specifically those that can be used for synthesising soft systems.

Implementation of LMs as sensors, electronic devices and interfaces may enable reactions in both liquid and solid states. Additionally, responsiveness to various stimuli and easy-to-functionalise interface of LMs make them ideal candidates for peculiar catalysis. The talk presents an overview on the synthesis and applications of LMs based materials.[1-3] This includes the applications of LMs in synthesising traditional functional systems and also illuminating the concepts in liquid states. The unique properties of LMs, which makes them promising materials for different applications will be discussed followed by relevant case studies.

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K.10 Hydrophilic Zwitterionic Polymer Coatings for Preventing the Adhesion of Bacteria on Medical Grade Polymers

Dr. Richard Kaner[1], Dr. Brian McVerry[2], Na He[2], Ethan Rao[2]
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Keynote Session 10, Skellerup & WSP, February 8, 2023, 9:10 AM – 9:50 AM

Nosocomial infections continually run rampant in US hospitals from implantable devices. The co-administration of antibiotics is typically used to reduce the amount of infection. However, antibiotic resistance and the proliferation of superbugs have motivated researchers to investigate antifouling polymers that resist adhesion of proteins and microorganisms. Unfortunately, the application of these polymers to the surfaces of medical devices often requires the use of pretreatment steps, exotic reaction vessels, and/or long reaction times that prohibit the widespread use of antifouling polymer modifications for implantable devices. We have developed a simple, one-step surface modification of several medically relevant materials using an anti-fouling zwitterionic polymer. Surfaces modified with the coating exhibit great antifouling properties of proteins when compared to the bare, unmodified surfaces. Furthermore, the modified surfaces resist the attachment and growth of several strains of bacteria and fungi, including superbug derivatives.

I2A.1 Enabling a Circular Economy: Carbon-Negative Fuel and Chemical Production by eliminating waste

Dr. Sean Simpson[1]
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2A | Commercial 1, Bay Trust Forum, February 8, 2023, 10:20 AM - 12:15 PM

The climate crisis is the most urgent challenge to mankind which can only be resolved via rapid action to drastically reduce waste carbon emissions. Carbon recycling technologies can transform above-ground carbon sources into sustainable fuel and chemical products. These technologies offer an industrial approach to both enable fuel and chemical manufacturing at its current scale, while achieving sustainability targets. Gas fermentation using carbon-fixing microorganisms is a fully commercial carbon recycling process technology that transforms waste carbon resources into sustainable fuels, chemicals and polymers at a scale that can be truly impactful in mitigating the climate crisis. LanzaTech is a pioneer and world leader in gas fermentation, having successfully scaled up the process from the laboratory bench to full commercial scale, with several commercial plants in operation and many additional facilities in construction.

Compared to other gas-to-liquid processes, gas fermentation offers unique feedstock and product flexibility. The process can handle a diverse range of high volume, low-cost feedstocks. These include industrial emissions (e.g., steel mills, processing plants or refineries) or syngas generated from any resource (e.g., unsorted and non-recyclable municipal solid waste, agricultural waste, or organic industrial waste), as well as CO2 with green hydrogen. These can all be converted into an array of fuels, chemicals or polymers either via traditional downstream chemical catalysis, or directly through the application of synthetic biology and metabolic engineering.

Direct synthesis of over 100 molecules via gas fermentation has already been demonstrated. In order to develop efficient production strains and accelerate time to market, tools such as automation, modeling and machine learning are critical. LanzaTech has established a first-of-its-kind biofoundry for fully automated, high-throughput engineering and screening of gas fermenting microbes. Through the application of synthetic biology to gas fermenting microbes, LanzaTech offers a sustainable, efficient route to directly produce numerous industrial chemical intermediates from waste carbon resources at scale.

I2A.2 Bringing ion beams out of the lab

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Most integrated circuits in today's electronic devices been exposed to ion beams many times their manufacturing to precisely dope and amorphise semiconductors.

Ion beam surface modification techniques are fantastic tools to control and engineer surface properties on most materials. Fast moving ions with kinetic energies beyond 1 keV can penetrate materials, modifying the chemistry and structure of the first nanometres to hundreds of nanometres. It can be used to control the charge transport properties of materials, modify a surface's mechanical properties (making it harder or softer), or create composite surfaces dotted with nanoparticles. In addition, while the energies involved are orders of magnitude larger than chemical and other physical techniques, ion beam techniques do not generally significantly increase the temperature of the sample to be modified, meaning that it can be used on temperature sensitive materials such as organic materials.

So why are ion beams not used more widely? And how could we realise the full potential of ion beam techniques?

In this talk I will take you along my scale-up and commercialisation journey, from modifying 1 cm^2 in batch processes to continuously modifying m^2 of materials as a manufacturer of catalyst coated membrane for water electrolysers. I'll highlight the key moments, findings, support and hurdles that have made that journey from a lab at GNS Science to co-found the start-up b.spkl.

2A.1 The KakaPore start-up: Capturing carbon dioxide

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We have developed a sponge-like adsorbent (MUF-16) that captures carbon dioxide with high efficiency. It can potentially reduce emissions at a range of scales, from large power plants and cement production to smaller geothermal electricity and fermentation processes. By using a solid-state adsorbent, we avoid the drawbacks incurred by traditional approaches such as amine solutions. It is readily interfaced with downstream carbon dioxide storage and utilization technologies.

KakaPore is a spin-out company charged with the commercialization of MUF-16. The name derives from the Kakapo, an iconic native bird of New Zealand. I will relay KakaPore's story to date.

2A.2 TasmanIon: Moving towards sustainable aluminium-ion batteries

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Decarbonising the world rests on solving the energy storage question. In the future, we'll require more lithium to construct batteries than currently available. Lithium-ion batteries (LIBs) are best suited for electric vehicles (EVs). The other industries that heavily rely on them (such as portable electronic devices, e-bikes, and stationary storage) should use newer and safer technologies.

Rechargeable aluminium-ion batteries are a promising alternative to meet the growing energy storage requirements1–3. TasmanIon will introduce a new energy storage device that is safer and more sustainable than the batteries currently on the market (lead-acid, nickel-cadmium, nickel metal hydride)4,5. It can be potentially more energy-dense than current LIBs, enabling significant weight benefits for multiple portable and stationary applications. Aluminium is the third most abundant material in the earth's crust – this means we are more sustainable than batteries that use metals from unethical sources (e.g., cobalt) or rarer metals.

The abundant raw materials enable the battery's lost cost profile. After each developmental phase spanned over the next few years, higher energy density batteries will be built for advanced applications such as the aviation industry. The current energy density of TasmanIon's AIB is comparable to the non-lithium batteries in the market6,7. It also can replace LIBs in sectors prioritising safety over high energy density. In the coming years, AIBs will create their niche in the battery industry and eventually move toward the EV market after further development!

TasmanIon is a university spinout company based on the core IP generated at Victoria University of Wellington.

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2A.3 Effect of processing conditions on suspension polymerization reaction of molecularly imprinted adsorption media

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Molecularly imprinted polymers (MIP) is a class of novel material where a polymer mixture is polymerized around a compound, e.g. a trace contaminant or valuable compound, resulting in an adsorbent which is specific for that compound. At present, MIPs have only been applied on the laboratory scale as a separation media, so MIP production is mostly carried out on the small-scale using bulk or precipitation processes, and typically have small particle sizes in the micro- or nanometer range.

Suspension polymerization involves polymerizing the MIP as droplets in a solvent (dispersed phase) in an immiscible or partially immiscible continuous phase such as water. This enables larger MIP resin beads to be produced which are suited for large scale, high throughput adsorption columns due to their lower pressure drop. MIP production using this method is also easier to scale up due being able to readily control reaction rates.

In this work, suspension polymerization of MIP specific for catechin hydrate was carried out using different mixtures of two solvents as the dispersed phase with water as the continuous phase. Using identical reactor conditions, the effect of solvent ratio on size distribution, resin morphology, and adsorption characteristics was investigated. Overall, an increase in solvent composition that increases its viscosity results in larger droplet sizes, increasing the maximum MIP particle size, while maintaining particle density and reducing surface area.

2A.4 A scalable solution-processed organic thermoelectric generator with record high thermocouple density

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Conversion of otherwise wasted low-grade heat (< 100°C), into electric power by organic thermoelectric generators (TEGs) is seen as a promising solution to supply energy to the growing number of microelectronics and sensors in the Internet of Things. Organic semiconductors (OSC) are particularly advantageous active materials for TEGs, due to their earth-abundance, tunable electronic properties and solution processability, yet only a few examples of organic TEGs exist in literature due to the limited library of high-performing n-doped OSCs[1]. Herein, we demonstrate a TEG made with p- and n-type legs that are both organic, based on poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS) and a high-conductivity n-type ink, poly(benzimidazobenzophenanthroline):poly(ethyleneimine) (BBL:PEI)[2]. The mixed ion-electron conducting films resulting from the BBL:PEI ink exhibit outstanding conductivities compared to other n-type OSCs and demonstrate excellent thermal, ambient, and solvent stability, thus making the ink an ideal choice for atmospheric fabrication techniques. The planar TEG architecture in this work leverages scalable ink-jet and spray-coating deposition techniques along with an ultra-thin parylene substrate, resulting in a device capable of taking on a rolled compact conformation, thereby achieving a record high thermocouple spatial density. The high-performing thermoelectric inks along with the compact design is here implemented in a proof-of-concept 4-legs OTEG capable of supplying 0.15 µW/cm² at ΔT=50K.

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2A.5 Wet-printing of Conformable and Stretchable Conducting Polymer Microelectrode Arrays for Gastric Slow Wave Recording

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Bioelectrical slow wave activity is a fundamental physiological event in maintaining the normal motility of the stomach and intestine. Dysrhythmias of slow waves lead to several major digestive disorders. High-resolution electrical mapping arrays have been used to investigate pathological slow wave abnormalities. However, conventional electrode substrate materials are opaque with high mechanical modulus, which leads to non-compliance and mechanical mismatch with the soft and deformable gut tissues. In contrast, conducting polymers (CPs) are well suited for bioelectronics applications due to their biocompatibility, tunable electrochemical and mechanical properties, mixed conductivity (ionic and electronic) and solution-processable fabrication.

In this work, we present the fabrication of highly stretchable and transparent conducting polymer PEDOT:PSS electrode arrays on stretchable polymeric substrates using a novel wet-printing technique. The fabricated electrodes demonstrated superb stretchability of more than 800% while remaining conductive. Remarkably, they are strain insensitive at lower strains with only 25% resistance increase at 100% strain. Such electrodes are perfect candidates for measuring the electrophysiological signals where muscle contraction and relaxation are involved.

The performance of the CP electrodes for the gastric slow wave recording was experimentally validated in a porcine model, against a previously validated Au-plated reference array. Slow wave activities were successfully picked by these electrodes with high amplitude and signal-to-noise ratio, and comparable frequency to the reference electrode array. Further adjustments of the deposition parameters and material composition will be investigated to further improve the performance of the electrodes.

I2B.1 Microfluidics at the interface of plants and pathogens

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2B | Bio 2 – Nanomedicine and agricultural applications, Skellerup, February 8, 2023, 10:20 AM - 12:15 PM

Fungi and their counterparts, the oomycetes, play an important role in the cycle of life as they efficiently decompose dead and decaying organic matter. Through this crucial role in the nutrient cycle they influence the well-being of human populations on a large scale. This is in contrast to certain species, which actively feed on living organisms, thus leading to pathogenic growth affecting both plants and animals.[1] Climate change, emerging drug resistance and travel and commerce induced world-wide spread of pathogens are all driving the need to better understand the interactions of pathogens with plants. In this paper I will summarize the microfabricated platforms we have developed to assist in the study of chemical, mechanical and electrical interactions between pathogens and plants, as well as how these can be used to investigate new bio-control strategies.[2] Spanning from artificial leaf substrates[3] and RootChips[4] to lab-on-a-chip devices used to study force generation[5], electrotaxis[6] and turgor regulation[7] in zoospores, the paper will touch upon the use of these systems to provide insight into diseases such as Kauri Dieback and Myrtle Rust, as well as plant responses to stress in general.

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I2B.2 Metabolic labelling as a novel approach for targeting the gastrointestinal tract

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2B | Bio 2 – Nanomedicine and agricultural applications, Skellerup, February 8, 2023, 10:20 AM – 12:15 PM

We have been concerned with the interaction of complex lipid particles with cells and trying to understand how on the one hand the underlying structure of the particle may influence their interaction with cells such as vascular endothelial cells, and on the other hand how they may be 'forced' to interact with cells using antibody-free cellular Velcro approaches in the gut using metabolic labelling and click chemistry. For the former we have been using simple models to mimic arterial and vascular flow in formats that offer the opportunity for additional in situ analytical techniques. The latter approach is shaping as an interesting option for localizing particles or other delivery vectors to specific regions of the gut.

2B.1 Studying the growth of oomycetes in an oxygen gradient on chip

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Oomycetes are fungal-like pathogenic microorganisms that can cause disease in many plant and animal species. These diseases impact ecosystems with loss of biodiversity, and in the agricultural, horticultural, forestry and aquaculture sectors cause huge economic losses[1]. They infect their hosts via infection structures and invasive cells called hyphae. The hyphae break down host tissue and absorb the released nutrients[2]. The energy required for growth and infection comes from oxidative respiration, despite the fact that the infection structures and hyphae may be exposed to oxygen concentrations as low as 1 – 2% in and around the host[3]. Pathogenic fungi, which utilize similar infective strategies, have been shown to sense and adapt to these hypoxic conditions, significantly altering their gene expression[4]. There are as yet no reports of how oomycetes respond to low oxygen concentrations. With a view to investigating this, we are developing oxygen sensor chips that expose oomycetes to oxygen gradients. Made from gas-permeable polydimethylsiloxan (PDMS), the chips comprise a central channel along which hyphae extend and two side channels, one on each side of the central channel. These are filled with oxygen or nitrogen that diffuses through the PDMS. This creates an oxygen gradient in the central channel that can be measured with the hypoxia-sensing dye Pt(II) meso-tetrakis(pentafluorophenyl)porphine (PtTFPP) embedded in PDMS[5]. Initial proof of concept experiments indicate that hyphae of the oomycete Achlya bisexualis are able to grow on the chips, sense oxygen concentration and orient their direction of growth toward the high oxygen side of the main channel.

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2B.2 Targeted nano-formulations in agriculture: Lessons from medicine

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Pharmaceutical excipients vary widely in function, being used as absorption enhancers, emulsifiers, preservatives, and sustained release matrices. Here the FDA-approved excipient, Poloxamer P188, is explored as a bioactive excipient in the wheat rhizosphere and contrasted with the natural osmolyte, glycine betaine. The P188 triblock copolymer self-assembles into 5.5 ± 0.3 nm micelles whose size does not vary significantly when encapsulating hydrophobic cargo, such as the plant metabolite quercetin [1]. Column transport studies demonstrated loaded P188 micelles delivered cargo intact, supporting assessment in plant studies. Wheat seedlings were grown in a sand matrix for 14 days, subjected to 8 days of simulated drought, and then recovered for 7 days. To better represent wheat grown in drought-prone regions, seeds were inoculated with a model rhizobacterium, Pseudomonas chlororaphis O6 (PcO6) which has been shown to improve drought tolerance through root colonization [2]. Seedlings were treated separately with 0.2 mmol P188 or 10 mmol glycine betaine per kg of sand matrix, or with the combined nano-formulation [3]. The quantum yield of photosystem II, total growth of plant mass, and relative water content under drought were measured. Both P188 and the P188 / betaine nano-formulation increased total above ground plant mass relative to the control, while the inclusion of betaine alone suppressed tissue growth and photosynthetic activity during periods of simulated drought but improved performance during recovery. P188 addition resulted in significantly higher relative water content in wheat under drought, suggesting activity as a synthetic osmolyte that resists sorption to soil components while carrying additional cargo intact through the rhizosphere.

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2B.3 Eco-friendly nanocarriers actualise biomolecule agrochemicals in crop production

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2B | Bio 2 – Nanomedicine and agricultural applications, Skellerup, February 8, 2023, 10:20 AM - 12:15 PM

The agricultural nanobiotechnology is prompting rapidly to tackle the increasing demand of food productivity against the loss of arable land and the activated movement of plant pathogen carriers due to global warming. Introduction of nanotechnology will afford effective, environmental, and economic solutions to actualize the new-generation agrochemicals for eco-sustainable agricultural production. [1] The nanoparticle-biomolecule hybrids are expected to replace the conventional toxic agrochemicals in the counteraction towards the loss of crop yield due to pests and pathogens with minimised impact to the ecosystem sustainability. [2] The nanoparticles will play an essential role in the agrochemical formulations by protecting the vulnerable biomolecules, such as nucleic acids, peptides, proteins, and metabolites, from the degrading environmental factors. Aiming to advance the research and development of the nanoparticle-biomolecule agrochemicals, expand the awareness of nanotechnology applications in agricultural production, and stimulate communication on this relatively new field from the elite audiences with broad nanotechnology background, we hereby introduce some typical nanoparticle-biomolecule hybrids as potential agrochemicals, including our own ground-breaking outcome, [3,4] and propose the criteria and strategy of the industrialisation.

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2B.4 Fabrication and characterisation of drug-eluting bioabsorbable surgical sutures

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2B | Bio 2 – Nanomedicine and agricultural applications, Skellerup, February 8, 2023, 10:20 AM - 12:15 PM

Sutures are the most popular surgical implants in direct contact with the wound, making a suture an ideal device for local drug delivery [1]. Despite the variety of commercial sutures available, none have the capacity to maintain their mechanical strength while delivering efficient anti-bacterial properties [1]. This study uses curcumin as an alternative to replacing chemical drugs, particularly antibiotics. Unlike antibiotics, curcumin is a natural product extracted from the common spice turmeric. It has anti-bacterial, anti-inflammatory and antioxidant properties [2]. The use of curcumin as part of a suture drug delivery system is an exciting new field. This study aims to produce a microsphere-embedded surgical suture as a controlled drug delivery system to facilitate wound healing. Firstly, curcumin-loaded microspheres were produced by the solid-in-oil-in-water emulsion method [3]. Subsequently, the curcumin-loaded microspheres were melt-extruded with biomaterials polycaprolactone (PCL) and polyethylene glycol (PEG) to obtain bioabsorbable antibacterial surgical sutures. During the microsphere production, it was found that the higher concentration of the water phase, the smaller the particle size became. The melting temperature, glass transition temperature and crystallisation temperature of microspheres-loaded polymeric sutures were observed at 56°C, -69°C and 30°C, respectively. Additionally, the suture sample displayed a smooth surface and possessed excellent tensile strength, which ascribed to the miscibility of PCL/PEG with curcumin-loaded microspheres. We hypothesize that our product will be biocompatible and able to accelerate wound healing.

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2B.5 Raman spectroscopy and chemometric analysis in phytoplankton monitoring

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Tracking phytoplankton health is crucial in monitoring nutrient availability in the environment as it forms the base of the aquatic food. In addition to environmental monitoring this is important in a range of applications such as aquaculture industry, pharmaceuticals and biofuels. Raman spectroscopy has long been suggested as a potentially fast and sensitive method to monitor phytoplankton abundance and composition in marine environment. Herein, the taxonomic differences, cell viability and growth phase characterization of several species of phytoplankton were investigated using NIR confocal Raman microscopy and excitation-emission fluorescence spectroscopy. The data was analyzed using principal component analysis (PCA) in combination with parallel factor analysis (PARAFAC). Subsequently, partial least squares discriminant analysis (PLS-DA) was used to classify the respective Raman and fluorescence data sets. [1] Our results demonstrate high cross-validation and prediction accuracy for different growth phases, taxonomic groups and cell viability. Findings of the current study illustrate potential for future developments of NIR Raman and fluorescence-based systems for use as label free, highly specific in-situ method in remote water sensing.

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I2C.1 Ionic liquid systems: exploring partial charges, charge transfer and polarizability.

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2C | Energy storage, electrolytes and ionic liquids, WSP, February 8, 2023, 10:20 AM - 12:15 PM

Ionic liquids (ILs) are of substantial interest for industrial applications, electrochemical devices (batteries) and as specialist engineering materials. There is a growing interest in the underpinning structural and dynamic properties of ILs, often facilitated through classical molecular dynamics (MD) simulations. For ILs understanding and accurately recovering the charge based interactions is vitally important. Moreover, the predictive and explanatory power a MD simulation is linked to the quality of the underlying force field.

Focusing on the widely employed [C4C1im][NTf2] (1-butyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide) IL we have considered the impact of different methods of determining the charge distribution,[1] identifying the ADCH charge model [2] as a good compromise between electrostatic potential and density based models. Within ILs charge transfer is known to occur, the standard approach is to uniformly scale all charges, however this approach may not always be suitable and we have developed an interpolation method for determining atom-wise scaled partial charges. Simulations based on atom-wise scaled charges have been compared to uniformly scaled and fully polarisable (Drude particle) simulations. The impact of not scaling the Van der Waals well-depth, and neglecting to employ a temperature grouped thermostat on fully polarisable (Drude particle) simulations has been examined.[3] Overall, we find that small changes in the charge description and polarisable methodology can have a significant impact on some properties while leaving others essentially unaffected.

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I2C.2 Tools for the search of new organic active materials for new redox flow batteries

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2C | Energy storage, electrolytes and ionic liquids, WSP, February 8, 2023, 10:20 AM - 12:15 PM

Due to the characteristics of flow batteries, this technology is ideally suited for low-cost storage in the range of a few hours and thus for load balancing as stationary storage in grids with high amounts of renewable energy [1]. Today, a large number of different active materials for flow batteries are known, although only a few have been commercialised [2]. Basically, the energy supply and thus also the required storage should be sustainable, i.e. not cause resource problems and not be harmful to humans and the environment. A potential for a huge range of possibilities is offered by organic active materials, which should be used especially in aqueous solutions. Due to the immense possibilities, classical synthesis and testing is extremely lengthy and costly. An alternative can be model-based high-throughput screening, where by simulating the properties of active materials in the electrolyte and the battery itself, computer-based simulations can be used to conduct the search.

The SONAR project is an EU-funded project in which 7 different institutions from the EU, Switzerland and Australia are developing a high-throughput screening method capable of finding new active materials for redox flow batteries. The principle is a serial coupling of different size scales, combined with molecule generation and machine learning. The chemical structure of a candidate is generated by a molecule generator and then its atomistic properties, kinetics, side reactions and cell properties are iteratively calculated with exclusion criteria.

In this talk we will give an overview of 2 years of research in this project in the areas of machine learning for high throughput screening, DFT based quantum mechanics modelling, kinetics Monte Carlo methods for meso-scale, 0D cell modelling, 3D cell modelling, stack modelling and techno-economics.

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2C.1 Interface Stabilization as a Key for Promoted Safety and Energy Density of Nickel-rich Cathode Material-based Lithium-ion Batteries

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2C | Energy storage, electrolytes and ionic liquids, WSP, February 8, 2023, 10:20 AM - 12:15 PM

Our society is being electrified with battery-of-things (BOT) for carbon neutrality. The demand for higher energy density and high safety of lithium-ion batteries (LIB) is then continuously increasing for longer range use of battery-powered advanced electronics, e-mobilities including electric vehicle and ESS, and for the safety of consumers, respectively. Strategies to increase battery energy density are to use higher capacity cathode active materials such as Ni-rich NCM and the charge of a battery to higher voltages than conventional 4.2 V. Challenges for battery safety are to innovate electrolyte technology from the flammable state-of-the-art liquid electrolyte to flame-retarding to nonflammable liquid electrolytes that provide as well a good solid electrolyte interphase (SEI) at the surface of both anode and cathode and therefore a good performance and cycle-life of a LIB. Our group has been designing and inventing functional electrolyte components and interfaces of anode/cathode materials for advanced LIBs, offering a significant improvement in the interface stability and performance, with respect to conventional ones. In this talk, I will present our recent progress on the advanced electrolyte- and binder-induced interface stabilization strategies of anode/cathode materials for safer and outperforming LIBs. A basic understanding of the mechanisms of performance improvement or failure will be discussed.

2C.2 Polysulfide Sieving Strategy through Tunable Ultralight Catalytic Interlayer for Stable Li-S Battery

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2C | Energy storage, electrolytes and ionic liquids, WSP, February 8, 2023, 10:20 AM - 12:15 PM

Lithium-sulfur (Li-S) batteries are attracting attention as next-generation energy storage devices beyond Li-ion batteries. However, despite being intrigued with the merits of high-performance, it has not progressed to practical applications due to limitations and complexity in terms of the insulative nature of sulfur and its volume changes. Worse is the multistep electrochemical conversion of sulfur during cycling to form a series of polysulfides (PSs) that carry different properties along with the “shuttle effect” making the operation of Li-S cells vulnerable. Here, we report a feasible strategy to effectively suppress polysulfide and selectively control ions transport applying a new-type aerofilm membrane for practical Li-S batteries. Catalytic hybrid aerofilm interlayer (HAI) consisting of a sulfonated tetrafluoroethylene (S-PTFE) and tunnel structured manganese dioxide nanowires suffices physically shield and sieve polysulfides through sulphophilicity polymer within the gaps of manganese dioxide layers while also impart chemical anchoring and catalysis of Mn-O. The importance of the sieving strategy lies on the tunable layers possessing angstrom level channels of Mn-O, and the sulphophilic SO3– in S-PTFE, inducing selective ions transport control allowing the passage of Li+ ions while limiting anionic species; thus, a homogeneous Li-flux is generated preventing the Li-dendrite and self-discharge in Li-S cell. Such co-operative synergetic effects of the HAI for the Li-S cells enabled a high discharge capacity of 1189 mAh g-1 at the end of the 500th cycle with a capacity retention of over 92.3 %, which indicated a 671 % improvement over sulfur battery without interlayer. Our strategy will offer new insights for developing a long-term and high-power Li-S battery.

2C.3 Tailoring charge transfer processes in organic radical batteries

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2C | Energy storage, electrolytes and ionic liquids, WSP, February 8, 2023, 10:20 AM - 12:15 PM

Nowadays organic batteries are among the most promising approaches in energy storage, e.g. due to their rapid charging, mechanical flexibility and sustainability.[1] Conjugated polymers were initially widely investigated in the scope of such organic batteries.[2] However, an unstable cell voltage over the desired capacity range prevents their broad application.[3] Alternatively, stable organic radicals such as the tetramethylpiperidinyl-N-oxyl radical (TEMPO) show highly promising properties,[4] yet lacking the desired conductivity.

In this joint synthetic-theoretical contribution, a new approach by combining stable N-oxyl-based organic radicals with a conductive polymer-based backbone is presented. Particular emphasis is set on the charge transfer (CT) kinetics assessed within the Marcus picture. The potential energy landscape was obtained at the CASSCF level of theory along efficient CT coordinates connecting the involved redox active species. Afterwards perturbation theory, namely NEVPT2, was applied to account for static as well as dynamic electron correlation. The chemical nature and length of the linker connecting the organic radical and the aromatic backbone as well as the ratio of the redox units were varied. Thereby, dependencies of the electronic couplings, thermodynamic properties and hence the CT rates on the structure of the organic radical system were revealed. By evaluating these structure-property relationships a deeper insight into the CT process is gained allowing the tailoring of new organic radical batteries with optimal charging/discharging kinetics. Very recently, this theory-driven approach led to the fabrication of the first battery from this new class of organic radical batteries with conducting backbone.

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2C.4 Towards predictive design of electrolyte solutions by accelerating ab initio simulation with neural networks.

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2C | Energy storage, electrolytes and ionic liquids, WSP, February 8, 2023, 10:20 AM - 12:15 PM

Electrolyte solutions play a vital role in a vast range of important materials science applications. For example, they are a crucial component in batteries, fuel cells, supercapacitors, electrolysis and carbon dioxide conversion/capture. Unfortunately, the determination of even their most basic properties from first principles remains an unsolved problem. As a result, the discovery and optimisation of electrolyte solutions for these applications largely relies on intuition/trial and error. The challenge is that the dynamic nature of liquid electrolyte solutions requires long simulation times to generate trajectories that sufficiently sample the configuration space; the long range electrostatic interactions require large system sizes; while the short range quantum mechanical interactions require an accurate level of theory. Fortunately, recent advances in the field of deep learning, specifically equivariant neural network potentials, can enable significant accelerations in sampling the configuration space of electrolyte solutions. Here, I provide an example of the successful application of this approach to the prediction the properties of aqueous sodium chloride solution.1 The implications for materials science more broadly will be discussed including identifying outstanding challenges and potential solutions.2

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2C.5 Ultrafast photoexcitation dynamics in ternary organic solar cells

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2C | Energy storage, electrolytes and ionic liquids, WSP, February 8, 2023, 10:20 AM - 12:15 PM

Organic photovoltaics (OPVs) are promising candidates for future renewable energy sources because of the advantages of organic semiconductor materials (OSMs), such as strong light-matter interactions, mechanical flexibility, and material tunability. One of the features of OPVs is using solution processes to form a unique active layer, bulk heterojunction (BHJ), for low-cost device fabrication. The basic BHJ consists of a binary mixture of electron donor and acceptor OSM; through the solution process, the BHJ can have a high degree of freedom in the change of compositions. Recently, ternary systems showed a promising approach to improving the device performance of OPVs. However, one of the challenges of ternary OPV is the system's complexity, leading to difficulties in understanding the details of the photocurrent generation process and the role of the third element. Here, we employ ultrafast spectroscopy techniques to investigate photoexcitation dynamics in two ternary OPV systems based on PM6:Y6, a high-performance non-fullerene binary OPV, with the third additives PC71BM and trans-bis(dimesitylboron)stilbene. By comparing the photoexcitation dynamics in the critical timescales between the binary and ternary OPV active layers, we reveal the impacts of the additives on exciton transport, which is the crucial mechanism for OPV. By establishing the relationship between ternary OPV's device performances, material compositions, functional layer morphologies, and ultrafast dynamics, our experimental results can provide insights to guide the material and component design for the ternary OPVs.

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I2D.1 Setting spins into a spin – single molecule toroidal systems

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2D | Nanoscale magnetism and characterisation, Downer, February 8, 2023, 10:20 AM - 12:15 PM

Since the discovery of a triangular Dy3 molecule showing a vortex arrangement of the individual DyIII spins [1-3], the concept of Single Molecule Toroics has led to exploration of other possible candidates based on 4f metal ions and Dy in particular. These will be discussed in further detail in the presentation. In addition to other cyclic arrangements such hexagonal Dy6 systems [4-6] examples incorporating 3d metal ions have helped to access larger molecules which are largely based on the idea of sandwiching 3d ions between two Dy3 triangles [7, 8]. The size of the triangles can also be varied by careful choice of the sandwiched structural motif as illustrated by the most recent and largest reported single molecule toroic synthesised and characterised by us at KIT [9].

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I2D.2 Nanoscale magnetophotonics

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2D | Nanoscale magnetism and characterisation, Downer, February 8, 2023, 10:20 AM - 12:15 PM

Nanoscale magnetophotonics unites the concepts from magnetism (switching, storage, steering) with light (energy, information, photochemistry) at the nanoscale (1). Our own exploration of this merger started some 10 years ago by conceiving nanoscale optical and magnetic antennas with magneto-optical properties dependent on optical resonances (2).
Today I highlight our recent work, were we employ plasmon nanoantennas to either funnel electromagnetic energy into ferrimagnetic films at the nanoscale assisting the ultrafast demagnetization (3), or construct hybrid plasmon-ferrimagnet nanoantennas for that (4). The produced architectures could also serve as the conceptually new high-resolution light incidence direction sensors or a platform with multistate demagnetization, potentially opening up for nanomagnetic neuromorphic-like ultrafast systems. We also show how adding nanoplasmonics allows to 'see' single molecule magnets with spectroscopy at ambient conditions (5). Finally, I discuss very intriguing prospect of 'spilling' materials properties (like electronic interband transition) outside the actual material by strongly coupling electronic and optical resonances in ferromagnetic Ni (6).

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2D.1 Atomic structure of metallic glasses studied by synchrotron-radiation X-ray diffraction, scanning tunneling microscopy and ab-initio molecular dynamics simulation

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The atomic structure of a Ni-Nb bulk metallic glass was studied by means of ultra high vacuum scanning tunneling microscopy [1]. Direct atomic structure observation was supported by MD simulation. Structural changes in a Zr-Cu-Ni-Al bulk glass-forming, relatively "strong", liquid alloy on cooling from above the equilibrium liquidus temperature studied by synchrotron radiation X-ray diffraction and first-principles molecular dynamics (MD) simulation are compared with those of a "fragile" Pd-Cu-Ni-P one [2]. According to the results chemical ordering forming Zr-Cu,Ni, Zr-Al and Zr-Zr atomic pairs takes place in the Zr-Cu-Ni-Al supercooled liquid alloy on cooling. However, here the change in the Zr-Cu,Ni peak area to other peaks area ratio is smaller than in case of the Pd-Cu-Ni-P alloy (Cu,Ni-P to other peaks ratio) in accordance with a lower fragility index of the Zr-Cu-Ni-Al melt. It indicates that fragility is a sign of instability of short and medium range order in fragile liquids.

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2D.2 New Developments in Electronic Structure Investigation: Combining APRES and Microscopy Solutions

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Momentum Microscopy is a new technology for comprehensive surface analysis, providing high energy and angular-resolved band structure mapping combined with advanced surface imaging capability. Extending this technology with laboratory-based instrumentation opens the possibility for detailed studies of new materials under well-controlled environments. The combination of a PEEM lens for surface microscopy and momentum microscopy, allows for small spot analysis in ARPES and chemically sensitive surface mapping. Here, we present the latest developments in analyzer technology, as well as key components for highly efficient laboratory-based surface analysis.

2D.3 Holistic approaches to Advanced Characterisation of Novel Materials

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Characterisation of Novel Materials can be a significant challenge due to the complex systems and interface interactions of the constituents, which can be at levels ranging from subnano - to micro-scale. The ability to holistically characterise these distributions and interactions has continued to grow in importance within CSIRO compared with conventional, bulk analyses.

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 Business Unit.

2D.4 Peering into the Computational Microscope: Insights from 3D printing through to virtual reality

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Most theoretical models of materials start out in the head of a materials scientist. A system is then constructed in the computer, and energetics or dynamics are calculated. This “hands-on” approach is being rapidly replaced by a “hands-off” approach where only the initial configuration is specified and the computer does the rest. These self-assembled structures provide a better experimental match without the constraints of our imagination but can be difficult to interpret.

In this talk, I will discuss the use of 3D printing, virtual reality and immersive 3D displays, all of which have provided key insights into the nanostructure of glassy carbon and formation mechanisms for soot and graphite. This will be followed by a demonstration of some virtual reality visualisations for attendees.

3D printing provided the key insight into the nanostructure of glassy carbon [1]. During preparation of the mesh for 3D printing, self-assembled models of disordered glassy carbon were found to possess a net-negative Gaussian curvature as well as a variety of non-sp2 defects that enable the ribbon structures seen in electron microscopy.

Non-contact atomic force microscopy, in collaboration with IBM-Zurich, enabled us to collect the first pictures of molecules that form soot in a flame [2]. We then developed multiscale models for these molecules to simulate the formation of a soot particle and a new, physically enhanced chemical mechanism was seen.

Virtual reality headsets enabled the formation of graphite to be observed from molecular dynamics simulations [3]. These matched the high-resolution transmission electron microscopy and X-ray diffraction studies also undertaken, revealing the role of screw dislocations in the formation mechanism of graphite.

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2D.5 Spin coating curved surfaces: simulation and experiments

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What do smartphone displays, solar cells, electronic circuit boards, and CDs have in common? They all tend to be flat, rigid structures. The reason for this feature relates to the fact that most of the manufacturing processes involved in the production of these objects have been optimized for flat, rigid substrates. The corner stone of these processes involves coating the substrate with a thin coating layer and a common technique, known for its effectiveness and low-cost, is spin-coating. To this day, spin-coating is only effective for flat substrates because it leads to non-uniformities on curved ones, [1].

In order to extend the applicability of spin-coating to curved substrates, it is important to better understand the interplay between substrate kinematics, substrate shape, and coating uniformity. In this talk, we extend theory of [2,3] and propose a simplified mathematical model based on the lubrication approximation able to capture the evolution of a thin liquid film on a rotating, curved surface, [4]. This model is validated against solutions of the full Navier-Stokes equations and offer the possibility to optimize the substrate kinematics to obtain a uniform film thickness. We also show corresponding experiments for the flow of a thin liquid film around a sphere subject to multi-axial rotation and illustrate how the process can be used in conjunction with photo-lithography to pattern curved substrates.

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I2E.1 Some new nanotechnologies for applications in cancer and immunotherapy

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Modern medicine is currently transitioning to a new paradigm of precision and personalized care, where patients will be comprehensively screened and monitored for the detailed molecular abnormalities that characterise their specific disease. In the past decade, nanotechnology has provided new tools with unprecedented power to comprehensively interrogate genetic, transcriptomic and epigenetic information. The Centre for Personalised Nanomedicine at UQ is focused on translating these new technologies into a clinical setting, whilst simultaneously developing the next generation of point-of-care diagnostic and therapeutic technologies to further empower the personalised and precision medicine approach. As part of a major National Collaborative grant funded by the National Breast Cancer Foundation ("Enabling clinical epigenetic diagnostics: The next generation of personalized breast cancer care", CG-12-07), our consortium recently published hundreds of epigenetic regions that are highly informative in cancer, as well as a unique (and simple to detect) epigenetic marker that appears to be universal for cancer1-3. These are now being validated in a real-time clinical setting, where comprehensive DNA, methyl-DNA and RNA information is collected in tandem and analysed. In this talk we will present data on the clinical translation of this approach, highlighting some of the positive impacts that such an approach can make on the "recovery trajectory" of cancer patients. Along with comprehensive DNA/RNA/methylated-DNA sequencing methodologies, several point-of-care nanotechnologies recently developed by our lab will be presented.e.g.,4-7. These include novel technologies for detecting circulating free DNA/RNA/methyl-DNA, circulated tumour cells, exosomes and protein biomarkers, as well as single-molecule read-out systems to monitor the immune system in real time.

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I2E.2 Chemical design of functional materials via surface-initiated polymerization

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Surface-grafted polymer thin films, which are commonly referred to as polymer brushes, have emerged as a unique class of surface coatings. Chain-end tethering polymers in close proximity using surface-initiated polymerization methodologies enforces a stretched conformation of the polymer grafts, which leads to several unique materials properties. Polymer brush films, for example, can be designed that are exceptionally effective in preventing biofouling, or which possess extraordinary low friction coefficients.

This presentation will highlight three recent discoveries from our laboratory that take advantage of surface-initiated polymerization reactions to generate polymer surface coatings with unique properties. In a first example, it will be shown how surface-grafted polymer films can be designed and prepared that display piezo- and pyroelectric properties, which is of great interest e.g. for energy harvesting applications. In a second example, it will be shown how, for a polymer film of a given thickness and composition, solvent uptake and swelling can be controlled, essentially by molecular engineering at the polymer brush – substrate interface. Since solvent swelling is essential to non-fouling and lubrication applications, this provides a new approach to engineer such properties. Finally, it will be shown how concepts from supramolecular chemistry can be harnessed to generate surface-grafted polymer films that potentially could be grown and removed in a repetitive, reversible manner.

2E.1 PEGylated liposome encapsulating nido-carborane: boron neutron capture therapy (BNCT) and in vivo trafficking study by PET imaging in animal models

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Boron neutron capture therapy (BNCT) is a binary radiotherapy based on nuclear reactions that occur when boron-10 is irradiated with neutrons, which results in the ejection of high-energy alpha particles. Successful BNCT requires the efficient delivery of a boron-containing compound to affect high concentrations in tumor cells while minimizing uptake in normal tissues. In this study, PEGylated liposomes were employed as boron carriers to maximize delivery to tumors and minimize uptake in the reticuloendothelial system. The water-soluble nido-carborane was encapsulated in the aqueous cores of PEGylated liposomes by hydrating thin lipid films. Repeated freezing and thawing increased nido-carborane loading by up to 47%. The average diameter of the prepared boronated liposomes was determined to be ~ 110 nm. When mice were irradiated by thermal neutrons, almost complete tumor suppression was achieved in tumor models injected with boronated liposomes. Two BNCT cycles spaced 10 days apart further enhanced the therapeutic antitumor effect. No notable weight loss was observed in the tumor models during the BNCT study. For in vivo tracking studies, nido-carborane was labeled with radioactive iodine at a radiochemical purity of >95%. At 1h post-injection, tumor accumulation was clearly detected by positron emission tomography (PET) imaging in the CT26 tumor models. In conclusion, PEGylated liposomes encapsulating high-content of nido-carborane were prepared simply by standard liposome preparation procedures. In the BNCT study, it showed a high tumor growth inhibitory effect. By efficient radio-iodination of nido-carborane, the tumor targeting efficacy of the injected liposomes was monitored non-invasively by PET/CT imaging.

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2E.2 Crystallins to Keratoplasties: Improving Biomimetic Corneal Stromal Materials

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The cornea is the outermost structure of the eye. An estimated 6-10 million people worldwide have blindness or a severe visual impairment attributed to corneal opacities[1]. For most, surgical intervention is the only effective treatment. However, due to the chronic shortage of cadaveric donor corneal tissue, only 1 in 70 people worldwide who require a corneal transplant will receive one[2].
The aim of this work is to develop and characterise corneal stromal equivalents to supplement the insufficient supply of cadaveric corneal tissue required for sight-restoring corneal transplant surgery.
A small animal study was conducted to test the biocompatibility of lens crystallin protein films developed for ocular therapeutics. Corneal health was scored according to a modified McDonald-Shadduck Scoring System, using indirect ophthalmoscopy and slit-lamp biomicroscopy. Animal study results show crystallin proteins are well tolerated in biological systems and resistant to degradation on the ocular surface.
Lens crystallin proteins will be used to augment electro-compacted type I collagen[3] and silk-based stromal equivalents systems[4]. Physiological-pressure inflation testing with ellipsoid modelling and compression testing will assess mechanical properties against human and porcine corneal tissue. The inflation testing rig has been constructed and allows for accurate pressure monitoring and image capture of corneas for analysis. Corneal stromal cells have been isolated and cultured in vitro, and stromal cell proliferation and gene expression profiles will be used to evaluate biocompatibility.
Current results show lens crystallin proteins to be a promising additive to stromal scaffolds to improve compatibility, longevity, mechanical strength, and overall fitness for purpose.

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2E.3 Bio-functionalization of titanium dioxide nanoparticles surface for controlling their cellular uptake in skin cells

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2E | Nanomedicine and functional biomaterials, Sigma, February 8, 2023, 10:20 AM - 12:15 PM

With the advance of nanotechnology, nanoparticles (NPs) have been continuously developed by desire for many applications such as imaging, biomedicals, and daily use products. It is quite difficult to avoid contact with NPs for example titanium dioxide NPs (TiO_2 NPs). Even TiO_2 NPs are widely used in sunscreen product, however; their safety issues for skin contact or inhalation are still in an argument [1-3]. If the NPs cannot penetrate to the skin, they will not be able to circulate to blood stream, accumulate in the body and cause side effects, ensuring them safety-to use. Therefore, this work aimed to modify TiO_2 NPs surface in order to inhibit their uptake into skin cells.

Inspired by protein corona study, bovine serum albumin (BSA), a major protein found in the blood stream was chosen to functionalize on the surface of TiO_2 NPs by physical adsorption. The protein attachment conditions were optimized by varying pHs and the condition giving the maximum BSA adsorption was applied. Then, the obtained particles (TiO_2-BSA NPs) were analyzed for physicochemical properties including size, zeta potential, morphology, UV absorption efficiency, and sun protection factor (SPF) capability compared to the unfunctionalized ones (TiO_2 NPs). Furthermore, both particles were investigated in terms of toxicity and efficacy in skin cells. Finally, their cellular uptake was studied quantitatively by ICP-MS and qualitatively by TEM and CLSM. The findings can be applied in NP based sunscreen products to reduce their internalization for consumer's safety.

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2E.4 In Vitro Trans-Blood Brain Barrier Delivery of Neurotrophin Loaded Nanoparticles to Address Neuronal Damage

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2E | Nanomedicine and functional biomaterials, Sigma, February 8, 2023, 10:20 AM - 12:15 PM

Neurodegenerative diseases comprise approximately 40% of annual incidences resulting in human disability and death. Most of the existing therapies focus on modifying disease progression and the symptoms of the disease without treating the neuronal cell loss. Members of the neurotrophin family of which brain-derived neurotrophic factor (BDNF) is the most abundant in the mammalian CNS, display trophic effects on a range of neuronal cells [1]. Delivery of such neurotrophic factors to patients has been challenging as neurotrophins are fragile molecules characterized by a short in vivo half-life (<2 min). The primary purpose of this research theme is to evaluate the efficacy of a therapeutic hybrid polymeric/lipid nanoformulation (NF) [2], to trespass the in vitro BBB and subsequently analyze its effects on an in vitro ischemic stroke model composed of human cortical neurons. In this regard, an in vitro BBB model was constructed, and once the integrity of the construct was confirmed, a dye-loaded NF was tested for its in vitro BBB trespassing ability. The results indicated that the NFs efficiently transported the dye across the construct. As the trans-BBB delivery ability of the NFs was established, further, BDNF-loaded NFs were prepared and tested for their therapeutic actions on the human cortical neuronal cells. The studies were performed in normal cell culture and hypoxic environments, the latter to mimic the hypoxia-induced neuronal damage and loss. Preliminary results have been encouraging in rescuing the damaged neurons. Further studies are underway.

2E.5 Real-Time Imaging of Nanoparticle Transcytosis in a Microfluidic Blood–Brain Barrier Model

Miss Yueying Cao[1], Guoying Wang[1], Xianlin Zheng[1], Jun Zhang[1], Jia Li[1], Bingyang Shi[1], Yiqing Lu[1]
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2E | Nanomedicine and functional biomaterials, Sigma, February 8, 2023, 10:20 AM - 12:15 PM

The blood-brain barrier (BBB) plays a pivotal role in maintaining homeostasis of the brain microenvironment, preventing pathogens and toxins from entering the brain [1]. Meanwhile, BBB also impedes the delivery of most therapeutic agents and poses a significant challenge for treating brain diseases [2]. Despite various approaches aiming to enhance BBB penetration have been investigated, the delivery efficiency is generally below 1% [3], suggesting in-depth knowledge of the BBB penetration process is critically required to overcome this barrier. Here we use lanthanide upconversion nanoparticles (UCNP) to visualize the transcytosis process through brain endothelial cells in an in vitro microfluidic BBB model. Incorporating cutting-edge strategies of high doping concentration and inert shell passivation to enhance the luminescence signal [4, 5], single UCNPs are clearly identified under microscopy imaging at 20 frames per second. This allows the movement of the UCNPs to be precisely captured with respect to the endothelial cells after being introduced into the vascular chamber of the BBB model. The integrity of the BBB is continuously monitored using a fluorescent dye, showing no compromise during the entire period of the imaging experiment. Thorough quantitative analysis of the UCNP trajectories, we successfully differentiate intracellular from intercellular penetration events based on their dynamic displacement against time for individual UCNP events. This is the first real-time observation of single nanoparticles crossing the BBB, which will help better understand the underlying mechanisms of BBB penetration and facilitate the development of new nanoparticle-mediated brain therapeutics.

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I3A.1 Waste as a resource… a rethink

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3A | Commercial 2, Bay Trust Forum, February 8, 2023, 1:15 PM - 3:30 PM

My talk will share Avertana's journey and some of the challenges we have faced in developing and scaling a world-first waste refining technology. It may be a disappointment to some that I won't be going into the minutiae of titanium dioxide primary particle and morphology control, let alone the measurement thereof! Rather, I will cover the associated themes of how we utilise existing mining and metal process wastes as a feedstock. What you will hopefully gain is shared insights into whether it is possible to break (or at least bend) the linear economic model. Avertana's approach has been to rethink how we can competitively make commodity products to serve existing markets by developing, and reducing to practice the science of deconstructing and remaking waste.

I3A.2 Facile dissociation of molecular nitrogen using lanthanide surfaces: Towards ambient temperature ammonia synthesis

Dr Franck Natali[1,3], Dr Anna Garden[2], Dr Jay Chan[3], Dr Casey Casey-Stevens[2], Dr Stephanie Lambie[5], Dr Ben Ruck[1], Professor Joe Trodahl[4]

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A combined experimental and computational study is reported on a hitherto unrecognised single lanthanide catalyst for the breaking of molecular nitrogen and formation of ammonia at low temperature and low pressure. We combine in situ electrical conductance and electron diffraction measurements as well as synchrotron-based experiments to track the conversion from the lanthanide metals to the insulating lanthanide nitrides. The efficiency of the conversion is then briefly discussed based on computational calculations (ab initio molecular dynamics and density functional theory), suggesting a molecular nitrogen dissociation pathway separate from that well established for transition metals. Finally, we show that exposure of the lanthanide surfaces to both molecular nitrogen and hydrogen results in the formation of ammonia.

I3A.3 Quantifying flow in bone with ultrasound and photoacoustic imaging

Dr Jami Shepherd[1], Caitlin Smith[1], Dr Guillaume Renaud[2], Dr Kasper van Wijk[1]
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3A | Commercial 2, Bay Trust Forum, February 8, 2023, 1:15 PM - 3:30 PM

The circulation of blood within bones is assumed to play a key role in bone health, healing, and in the progression of bone disorders. However, there is no appropriate technique to quantify blood flow in bone for use in routine clinical practice. Quantitative blood flow measurements in bone require invasive sampling of the bone tissue, which is clinically impractical. Magnetic resonance imaging, positron emission tomography, and optical methods have also been considered for this task. Unfortunately, MRI is limited to bone marrow only, PET suffers from poor spatial resolution, and optical methods are limited to superficial imaging depths. Further, none of these modalities provide information about the direction of blood flow in bone.

In this talk, I will present our work developing new techniques for imaging and quantifying blood flow in bone with ultrasound and photoacoustic imaging. First, I will describe how we overcome the limitations of conventional systems to image beyond soft-tissues into bone with ultrasound. Conventional methods approximate the entire human body as a fluid, which breaks down for bone. We account for the true wavespeed model in bone, allowing us to differentiate between soft-tissue, cortical bone, and marrow. Second, I will present our progress in quantifying blood flow in bone. We acquire hundreds of images over time, and apply post-processing to determine the magnitude and direction of flow ("vector flow") at each pixel in the image. Benchtop measurements in bone models as well as in vivo feasibility measurements will be presented.

3A.1 Rare earth nitrides: From the lab to the world

Dr William Holmes-Hewett[1], Dr. Jackson Miller[1], Dr. Franck Natali[1], Dr. Ben Ruck[1], Dr. Bob Buckley[1], Dr. Joe Trodahl[1]
[1]*Victoria University Of Wellington, Wellington, New Zealand*

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The rare-earth nitride series of intrinsic magnetic semiconductors is unparalleled in terms of its tuneable magnetic and electronic properties. The opportunities offered to both fundamental science and applications are also (some would say) unparalleled. Saturation magnetisation, coercivity and angular-momentum can all be selected by various choice of lanthanide ions, whose strong spin-orbit interaction and variously filled 4f shell make possible a continuous matrix of magnetic properties. The control of these properties has potential to solve outstanding problems in cryogenic data storage, on which the future of large-scale superconducting and quantum
computing hinges.

The current generation of cryogenic computers rely on memory systems using existing CMOS technology, which in most cases requires an inefficient link between the 4 K logic devices and the room temperature memory devices. Cryogenic-compatible memory based on Josephson-junctions can be housed at the same temperature as existing superconducting and quantum logic devices, if not on the same chip, with clear advantages. There are fundamental challenges to face before such devices are realisable, many of which are eased by the continuously tuneable magnetic properties of the ReN. In this talk I will give an overview of the journey our team has taken, from being among the first to grow these materials as thin films in 2006, through fundamental studies, through two generations of memory device prototypes and our current push into commercialisation. My talk will serve as an introduction and overview of the more detailed abstracts concerning rare-earth nitrides which are presented by students and postdocs.

3A.2 Boosting the Performance and Longevity of CO2 Capture and Conversion using Micro-nano Engineered Gas-Capturing Surfaces

Sami Khan[1], Yang Shao-Horn[2], Kripa Varanasi[2]
[1]*Simon Fraser University, Vancouver, Canada,* [2]*Massachusetts Institute of Technology, Cambridge, United States*

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As the intensity of severe climate events continue to magnify around the world, there is a growing need for materials that can expedite the capture and conversion of greenhouse gases. Previous research in the field of CO2 electroconversion (CO2RR) has focused on developing novel catalysts to enhance the activity and product distribution (selectivity). Copper has been studied widely, however even the best copper electrocatalysts are not immune from the competing hydrogen evolution reaction: the poor solubility of CO2 in water (~34 mM) limits the CO2RR current density, and hydrogen generation is favored if the aqueous CO2 concentration becomes locally undersaturated close to the catalyst during CO2RR [1,2].

We have developed specialized gasphilic CO2 traps that increases gas-liquid mass transfer and maintain supersaturated CO2 concentration around the catalyst during CO2RR. These novel gasphilic surfaces integrate hydrophobicity and nanotextures to capture bubbles and form a sheet of gas underwater which is called a plastron. When this plastron is placed proximal to both smooth and nanostructured copper catalysts during CO2RR, the current density is enhanced by 50% and maintained throughout the reaction. The plastron allows for quick replenishment of CO2 during the CO2RR reaction in the vicinity of the catalyst. As a result, there is an increased production of valuable carbonaceous products including ethylene, ethanol and propanol (by over 40%), as well as 60% reduction in hydrogen co-evolution.

This talk will conclude with a forward-looking perspective on the role of interfacial engineering in enhancing the performance and longevity of broader sustainable energy systems.

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3A.3 A High-Valent Organic Linker-Based Metal-Organic Framework for Selective Methane Capture

Dr Lujia (Luke) Liu[1], Zi-Zhong Zhang[1], Yiming Zhang[2], Dr Seok Lee[2]
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Methane is a potent greenhouse gas contributing to around 30% global warming.[1] One way to cut methane emissions is to capture methane from fixed emission sources. Coal-mine methane remains a challenging target because methane concentration is only 0.5% after ventilation.[2] As such, materials that can selectively adsorb methane are highly desirable.

Although research into selective methane capture is in its infancy, characteristics for optimal methane storage materials are well understood. Large-scale screening of over 137,000 hypothetical metal-organic frameworks (MOFs) suggests that the most frequent pore sizes among the top-performing materials are 4 and 8 Å, just big enough to fit one or two methane molecules.[3] However, most of these top-performers pillar-layered structures are synthetically challenging due to their tendency to interpenetrate and deform upon solvent removal.

To tackle this synthetic challenge, we designed a high-valent organic linker with geometry resembling a metal cluster used in MOFs. This unique linker produced a MOF with optimal structure characteristics for methane capture. Our preliminary data suggests that this material has a striking CH4/N2 selectivity over 10 and is among the two most selective methane adsorbents reported.

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3A.4 Antibacterial and Antiviral Solid-State Carbon Cloth Supercapacitor

Miss Sara Beikzadeh[1,4], Dr. Alireza Akbarinejad[1,4], Dr John Taylor[2], Professor Simon Swift[3], Professor Paul Kilmartin[1], Professor Jadranka Travas-sejdic[1,4]

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With the emergence of deadly viral and bacterial infections, the prevention of microorganisms spread on surfaces has gained ever-increasing importance. It has recently been discovered that capacitive materials can deactivate bacteria and viruses after being charged with a low voltage [1].

In this study, a new concept of antibacterial and antiviral supercapacitors is introduced. Here, we develop a simple, low-cost and flexible carbon cloth supercapacitor (CCSC) with highly efficient antibacterial and antiviral surface properties. CCSC can be charged at a low constant potential of 1 to 2 V. The charged CCSC uses the stored electrical charge to destabilize the electrokinetic properties of viruses and disrupt their infectivity upon virus contact with the surface, as well as disinfect bacteria through the membrane and wall electroporation. The optimized CCSC showed excellent electrochemical properties, including a capacitance of 4.15 ± 0.3 mF/cm2 at a scan rate of 100 mV/s, high-rate capability and electrochemical stability given by 97% retention of the initial capacitance after 1000 cycles. The CCSC showed excellent flexibility and retention of its full capacitance under high bending angles. The positively charged side of the CCSC devices yielded 6 log CFU reduction of Escherichia coli (gram-negative) bacterial inocula and 5 log reduction in PFU of HSV-1 herpes virus (an enveloped double-stranded DNA virus). This technology can be considered a new generation of environmentally friendly antibacterial and antiviral platform that provides a broad range of sustainable biocidal activities with lower power requirements.

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I3B.1 German-New Zealand: Green Hydrogen

Professor Sally Brooker[1], Dr Paul Jerabek[2]
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3B | Catalysis 2 - Hydrogen production and storage, Skellerup, February 8, 2023, 1:15 PM - 3:30 PM

This invited lecture will present:

a) An introduction to hydrogen, including a summary of its existing roles as a key industrial chemical and consideration of future roles.

b) An update on the development of the German-New Zealand green hydrogen research, networking and outreach centre, co-led by Dr Paul Jerabek and me, in partnership with Ngāi Tahu, and co-funded by the BMBF (Germany) and MBIE (NZ) for 5 years from 2021.

c) An introduction to the three German-NZ green hydrogen research projects recently co-funded by the BMBF and MBIE for 3 years, before briefly focussing on our one: 'safe cost effective H2 storage materials from NZ resources' with big team: 5 PhD and 3 Masters students, plus Aimee Kaio, Dr Linda Wright, A/Prof Nigel Lucas, Dr Anna Garden, A/Prof Michael Jack, A/Prof Jonathan Leaver, Dr Chris Bumby, A/Prof Alex Yip and Prof Peng Cao, co-led by Paul and me (HZH, Otago Uni, Awarua Runaka and Te Rūnanga o Ngāi Tahu, NZ Hydrogen Council, Unitec, Robinson Research Institute-Vic Uni, Canterbury Uni, Auckland Uni and MacDiarmid Institute).

d) Finally, brief consideration of some exciting German initiatives to accelerate their move to a hydrogen economy, and of some of NZ's advantages as we also look to shift to a suite of low-C and zero-C emission fuels, including hydrogen.

I3B.2 Metal Hydride Materials for Solid-State Hydrogen Storage Applications: Utilizing the Synergy of Experiment & Theory for Materials Design Challenges

Dr. Paul Jerabek[1]
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3B | Catalysis 2 - Hydrogen production and storage, Skellerup, February 8, 2023, 1:15 PM - 3:30 PM

Metal hydride materials present a safe, efficient and long-term storage option for hydrogen under mild conditions. They they will play an important role in the transition towards a carbon-emission-free energy economy due to their very high volumetric densities that even surpass cryogenically cooled hydrogen storage and thus provide attractive options for storing hydrogen for many stationary and mobile applications.

Deep understanding of (de)hydrogenation thermodynamics and kinetics of metal hydride materials is essential in order to allow targeted design of novel hydrogen storage materials and optimization of existing compositions tailor-made for specific application scenarios. To obtain the necessary insights, theory and experiment need to work closely together in order to fully leverage theory-experiment feedback loops.

To shed some light on the current and future challenges in this area, this talk will give an overview of metal hydride materials and their applications as well as the joint experimental and theoretical investigations by the Materials Design groups at the Helmholtz-Zentrum Hereon.

I3B.3 The Rocky Road Towards Earth-Abundant Metals in Photocatalysis – A Quantum Chemical Perspective

Dr. Stephan Kupfer[1]
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3B | Catalysis 2 - Hydrogen production and storage, Skellerup, February 8, 2023, 1:15 PM - 3:30 PM

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]

In this contribution, we investigate the accessibility of prominent – yet undesirable – excitation-state deactivation channels via the so-called metal-centred states of 3d metals using quantum chemical simulations in association with time-resolved spectroscopy. Based on the reliable description of photophysical and photochemical processes studied using state-of-the-art multiconfigurational methods and cost-efficient time-dependent density functional theory,[3] we present selected aspects of our theory-driven design concepts to drive the desired electron and energy transfer processes associated with catalytic turn-over. To this aim, the driving forces, electronic couplings as well as the reaction coordinates connecting the diabatic states involved in the light-driven process of interest are elucidated by means of our lately introduced external optimizer pysisyphus[4] and systematically tuned upon structural modification.[5,6] Finally, structure-property relationships are discussed in the context of a bio-inspired hydrogen-evolving photo-active dyad exclusively based on non-precious earth-abundant elements.[7]

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3B.1 Exploring the potential for water-based upconversion to enhance hydrogen production by photolysis

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3B | Catalysis 2 - Hydrogen production and storage, Skellerup, February 8, 2023, 1:15 PM - 3:30 PM

The response to the climate change crisis requires a radical shift from fossil fuels to achieve 'net zero' carbon emissions. Hydrogen (H_2) is an attractive alternative, however, production of "green" hydrogen fuel is limited by its high energy cost. The energy required to split water into hydrogen and oxygen via a photocatalytic system under standard conditions, is 4.915 eV. This is equivalent to the energy generated from one photon of ultraviolet light,[1] meaning that the amount of solar radiance that can be used to drive this reaction is greatly restricted. However, through the photon upconversion process of triplet-triplet annihilation (TTA), one visible light photon can be produced from two infrared photons, to yield the same energy output. Thereby allowing for a wider range of the solar spectrum to be utilised. It has been established that nanocrystal/organic sensitiser hybrid models are able to achieve efficient upconversion.[2] However, these systems are faced with two main challenges 1) for TTA to occur, all components must be in close proximity, and 2) triplets are quenched by oxygen. This work aims to combat these challenges through the development of a polymer encapsulated nanocrystal/sensitiser conjugated system.

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3B.2 Computational Recipes for High-Throughput Screening of Metal Hydrides for Hydrogen Storage

Dr. Kai Sellschopp[1], Dr. Paul Jerabek[1]
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3B | Catalysis 2 - Hydrogen production and storage, Skellerup, February 8, 2023, 1:15 PM - 3:30 PM

Green hydrogen will play a major role in the energy transition towards a cyclic economy for replacing fossil feedstocks in the chemical industry and for sustainable energy storage. Metal hydrides allow to store hydrogen in the solid state at ambient conditions. The development of new sustainable metal hydrides with the desired properties necessitates a deeper understanding of these materials as well as a high-throughput screening of interesting candidates. Computational studies with ab-initio methods deliver many of the properties relevant for discovering new metal hydrides, such as formation enthalpies, diffusion barriers, and electronic structure. However, all ab-initio methods rely on approximations and choices made by the researcher to reduce the computational effort, which are rarely reviewed. Therefore, this contribution assesses the accuracy of some of the most common of these approximations and choices, such as density functionals, dispersion corrections or inclusion of vibrational contributions, for a set of binary metal hydrides.

As a result, computational recipes for metal hydrides are developed, which can be employed in high-throughput screening of new candidate materials as well as in in-depth studies of material properties. The computational recipes consist of the settings (ingredients) and also the workflow (instructions) to obtain desired properties. Developing a cookbook of computational recipes will enable a partially automated search for new materials. Furthermore, it will make it easier for any materials scientist to dive into the intricate task of computing the properties of metal hydrides, just as a regular cookbook makes it easier for anyone to prepare a tasty dish.

3B.3 Ion beam synthesis of metastable, high temperature transition metal carbides at room temperature

Dr Holger Fiedler[1], Niall Malone[1,2], Dr David R.G. Mitchell[3], Dr Mitchell Nancarrow[3], Prof Geoffrey I.N. Waterhouse[2,4], Dr John Kennedy[1,4], Dr Prasanth Gupta[1,4]

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3B | Catalysis 2 - Hydrogen production and storage, Skellerup, February 8, 2023, 1:15 PM - 3:30 PM

Ion beam synthesis is a high energy technique, suitable for the formation of metastable, high temperature materials at room temperature. On the example of MoC, the formation of phase-specific MoC nanoparticles at room temperature using our ion beam selection principles are demonstrated. Monte-Carlo simulations provide guidelines for the ion beam parameters to enable the formation of predefined stoichiometry, while the thermal spike model is used to estimate the localized temperature during the collision cascade. We demonstrate the formation of phase-pure η-MoC nanoparticles with a diameter of 10 nm after implantation of 9×1016 at.cm-2 Mo+ with an acceleration energy of 30 keV into glassy carbon. In agreement with the counterintuitive conclusion based on the thermal spike model, higher energies lead to reduced localised heating during ion implantation which enables the formation of small metastable γ'-MoC nanoparticles after 60 keV Mo+ implantation into glassy carbon. Simulations demonstrate that due to the high Mo content, the β-Mo2C phase is only accessible by ion implantation of Carbon into Mo. We compared the catalytic activity of the formed phases for the hydrogen evolution reaction (HER) and demonstrate that the Mo phases have an improved catalytic activity, following the sequence η-MoC < γ'-MoC < β-Mo2C. This agrees with the previously reported HER activity of these phases [1], complementing the material characterization by transmission electron microscopy, x-ray photoelectron microscopy and Rutherford backscattering [2]. The described methodology and ion beam selection can be extended to fabricate and modify other materials (E.g. III-V semiconductors [3]).

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3B.4 Synthesis of nano-structured Li4Ti5O12 via a superhydride-driven wet chemistry method as a highly sustainable anode material for lithium-ion batteries

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3B | Catalysis 2 - Hydrogen production and storage, Skellerup, February 8, 2023, 1:15 PM - 3:30 PM

Lithium-ion batteries (LIBs) are at the forefront among existing rechargeable battery technologies, which have achieved great success in portable electronics and even recently electronic vehicles. However, lithium-ion batteries are confronted with several issues in terms of safety and cycle life. Spinel Li4Ti5O12 (LTO) has attracted widespread research attention as an anode material in LIBs owing to its intrinsic safety, long cycle life, and structural stability. In this paper, nanostructured LTO with a spinel structure was successfully synthesised via a superhydride-driven wet chemistry approach. The annealed powder was characterised via XRD, TEM, SAED, SEM, and XPS. Spinel LTO was tested as negative electrode material in a lithium-ion battery. The electrochemical performances were characterized by using CV, EIS, and galvanostatic cycling. The LTO exhibits good rate capability when assembled into half cells and tested in the 1.0 to 2.5 V range. It exhibits a reversible discharge capacity of 96.8 mAh g -1 at a 2C rate while maintaining a Coulombic efficiency of 99.9% after 100 cycles. The overall resistance of the LTO/Li cells at 25 °C is only 35.5 Ω, suggesting a low impedance of the LTO/Li interfaces. The effect of Li-loading, calcination time, and temperature on the structure and properties of LTO was also investigated.

I3C.1 Introducing Disorder and Magnetism into Topological Materials

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3C | Topological, quantum and superconducting materials, WSP, February 8, 2023, 1:15 PM - 3:30 PM

Recent theories predicting that disorder in certain topological insulators may not destroy the topological effects [1]. On other hand, a new theoretical study demonstrated a topological transition in Sb2Te3 [2]. In this talk, I will explore the electronic properties of disordered topological insulators as a result of ion irradiation.

In the first part of my talk, I will discuss the role of porosity in the enhancement of the phase coherence length in the topological insulator, Bi2Te3. It has been known that improved topological transport can be realised by increasing the surface-to-volume ratio, and previous research has explored ultra-thin samples and nanowires. In this work, porosity as result of Ne ion irradiation was used to increase the surface-to-volume ratio. The phase coherence length doubled in the porous samples. This increase is likely due to the large Fermi velocity of the Dirac surface states. Our results show that the introduction of nanoporosity does not destroy the topological surface states but rather enhances them, making these nanostructured materials promising for low-energy electronics, spintronics and thermoelectrics [3].

In the second part of the talk, I will discuss how we can directly control the topological electronic states in the topological insulator, Sb2Te3. This is done using an ion beam to drive a quantum transition between crystalline and amorphous structures. Our experimental results show that Sb2Te3 represents a promising platform to switch on and off topological properties.

Finally, I will discuss the electronic and magnetic manipulation of materials such as SnTe as a result of ion irradiation with 3d transition metals.

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I3C.2 The Topological Transistor as a Low-Voltage Switch

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3C | Topological, quantum and superconducting materials, WSP, February 8, 2023, 1:15 PM - 3:30 PM

The impending end of Moore's Law has prompted a search for a new computing technology with vastly lower energy consumed per operation than silicon CMOS. The recent discovery of topological phases of matter offers a possible solution: a "topological transistor" in which an electric field tunes a material from a conventional insulator "off" state to a topological insulator "on" state, in which topologically protected edge modes carry dissipationless current. This electric field-tuned topological transition has advantages over current MOSFETs: (1) Due to the combined effects of Rashba spin-orbit interaction and electric field control of the bandgap, the topological transistor may switch at lower voltage, overcoming "Boltzmann's tyranny"[1], and (2) true electric field-controlled switching opens the possibility of using the full power of negative capacitance structures as an electric field amplifier to achieve further reductions in switching voltage[2]. We have studied thin films of Na3Bi grown in ultra-high vacuum by molecular beam epitaxy as a platform for topological electronic devices. When thinned to a few atomic layers Na3Bi is a large gap (>300 meV) 2D topological insulator, and electrical transport measurements demonstrate that the current is carried by helical topological edge modes over millimeter-scale distances[3]. Electric field applied by proximity of an STM tip can close the bandgap completely and reopen it as a conventional insulator[4] demonstrating the basis of electric field-switched topology.

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I3C.3 Materials Nanoarchitectonics: The World-Smallest Car Race to Artificial Brain

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3C | Topological, quantum and superconducting materials, WSP, February 8, 2023, 1:15 PM - 3:30 PM

Functionality of materials appears when multiple matters interact with each other. In the case of single molecules, variety of properties and reactions emerges when the molecule is in touch with another molecules, substrates under surrounding environments. By controlling and designing a molecule and surrounding conditions, we would be able to let the molecule work as we intend. To establish such technology, the world-smallest nanocar race was organized in 2022. We participated in the event and successfully drove our nanocar on a gold surface, resulting in winning the race. Our nanocar was designed to show excellent stability but was difficult to be synthesized in solution, so we used materials nanoarchitectonics to complete the synthesis on a gold surface before the race.

Large-scale materials nanoarchitectonics also led us to discover the emergence of brain-like information processing only using non-biological materials. Since we can find various memristive behavior in nanoscale switching elements, we constructed large-scale assembly of memristive elements connected with each other through metallic nanowires, namely the nanowire network. Emergence of dynamics in the nanowire network enables learning, forgetting, and associatively recalling memories without control processing unit used in the present computers.

3C.1 Thin-film multilayers of the high-temperature superconductor YBa2Cu3O7 and manganates RMnO3

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3C | Topological, quantum and superconducting materials, WSP, February 8, 2023, 1:15 PM - 3:30 PM

Thin-film multilayers of metal-oxides exhibit a range of emergent, and potentially useful, properties [1]. These are the result of interactions across the interface, such as spin and orbital reconstruction, charge-transfer and phonon-coupling [2]. Multilayers of the cuprate high-temperature superconductor $YBa_2Cu_3O_7$ and rare-earth manganates $RMnO_3$ are a prime example [3]. They are of particular interest to us as when R is chosen such that the manganate exhibits charge-orbital ordering, multilayers exhibit a highly unusual insulating-to-superconducting transition (IST) driven by a magnetic (or electric) field [4-6].

Here, we present recent studies of these multilayer materials, which when taken together further confirm that the IST intrinsically results from a coupling between the cuprate and manganate layers. Spectroscopy has been a key tool in developing this conclusion, and here we present key x-ray absorption and Raman results.

A detailed explanation of the coupling between the cuprate and manganate layers remains a key challenge, in part frustrated by the complexity of these systems. However, it is also an opportunity to better understand and manipulate the superconducting state in the cuprates.

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3C.2 Zeeman Interactions in Rare-Earth Doped Nanocrystals

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3C | Topological, quantum and superconducting materials, WSP, February 8, 2023, 1:15 PM - 3:30 PM

Nanomaterials doped with rare-earth (lanthanide) ions have considerable potential for advanced technologies, from quantum computing to biomedical applications including imaging, nano-thermometry, photodynamic therapy.

There has been recent interest in using magnetic fields to modulate energy transfer between lanthanide ions in nanocrystals [1]. However, most investigations have not considered the details of electronic and magnetic energy levels. Applications development would be assisted by a better understanding of the magnetic splitting in nanocrystals. Though the particles are randomly oriented, we have recently shown that useful information may be obtained by Zeeman spectroscopy of rare-earth-doped nanoparticles [2,3].

In this work we combine high-resolution absorption and emission data of rare-earth doped nanoparticles measured at cryogenic temperatures with Zeeman data. This data allows an accurate analysis of the electronic structure of the rare-earth ions in the nanoparticles, and we discuss possible differences from the electronic structure in bulk crystals and the potential use of using magnetic fields to enhance performance in sensing applications.

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3C.3 Designing high-performance superconducting thin films using ion beam technology

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3C | Topological, quantum and superconducting materials, WSP, February 8, 2023, 1:15 PM - 3:30 PM

High-temperature superconductors with enhanced critical current density and reduced anisotropy are strongly desired for the manufacture of many devices proposed for sustainable energy production, transport, energy storage as well as medical applications. The intentional creation of non-superconducting phases independently of the existing microstructure through ion beam technology has proved to be a successful method for achieving high critical current performance in superconductors. The desired morphology of damage tracks can be achieved by selecting the appropriate type and energy of irradiating ion and the desired density and orientation by choosing the fluence and angle of irradiation respectively. Point defects created by irradiating the material with light ions like protons are good candidates for creating an isotropic enhancement and columnar tracks created by heavy ions like silver are proved to be excellent in creating highly enhanced performance at specific angles. These structures impact differently on the critical current at different temperatures, magnetic fields, and orientation of sample with respect to external magnetic field. This study investigates the impact of proton and silver irradiation over a range of temperatures of 20-77.5K, field of 0-8T and full rotation about one axis thus covering the parameter space of critical current anisotropy. In particular, at low temperatures and high magnetic fields relevant to applications like fusion reactors, we have achieved a factor of 2.6 isotropic enhancement over an already optimized and commercially superconducting tape. The knowledge gained will benefit the real applications in which wire will experience different temperatures and magnetic fields spanning a wide range of strengths and orientations.

3C.4 Reducing Thermal Conductivity in n-type Thermoelectric Oxides Using a Novel Cold Sintering Process

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3C | Topological, quantum and superconducting materials, WSP, February 8, 2023, 1:15 PM - 3:30 PM

Thermoelectric materials have the potential to ease the demand on fossil fuels by recuperating the waste heat released on mass during energy conversion processes. Foreman et al. report the amount of energy lost as waste heat as close to two thirds of the total energy we convert from primary energy resources. [1]
The current barriers for wide scale use of thermoelectric devices are cost and efficiency: the efficient materials like bismuth telluride are too costly, metal oxides are a much cheaper, less toxic alternative to tellurides but their efficiencies, particularly in the n-type materials, are much lower. However, in 2016 Zhilun Lu et al. [2] published the highest ZT (figure of merit) n-type metal oxide to date : $La_{0.15}Sr_{0.775}TiO_3$. By taking this composition and reducing its thermal conductivity via nano-sizing we can push the figure of merit even higher in order to be a competitive component for wide-scale-use thermoelectric devices. To achieve this we have coupled ionic liquid synthesis and a modified version of the recently proposed Reactive Cold Sintering Method to retain the small grain sizes achieved from a wet chemical synthesis within a highly dense final product.[3]

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I3D.1Thermoluminescence of MgAl2O4 and ZnAl2O4 Spinels

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3D | Optical materials 2, Downer, February 8, 2023, 1:15 PM - 3:30 PM

Spinels present large compositional diversity and property tunability and thus are of interest to many technology fields. The cubic structure and broad optical transparency associated with a large band gap make these materials particularly attractive for optical applications [1]. The capacity of accommodating relatively large amounts of anti-site defects make them good candidates for applications involving radiation damage. This work focuses on Mg and Zn aluminate spinels.
MgAl2O4 and ZnAl2O4 powders were prepared by the co-precipitation method and calcined at 900 oC for 2 hrs. in air. Natural and artificial crystals were also investigated. Structural characterization was executed by X-ray diffraction and Raman spectroscopy. Radioluminescence (RL) under X-ray excitation was recorded towards the identification of all luminescence centers present in the different materials. RL measurements revealed that both spinels presented a broad band peaked at ~400 nm attributed to antisites and other defects, and bands attributed to Cr3+, Mn4+ and Mn2+ impurities. Thermoluminescence (TL) spectroscopy measurements up to 400 oC were executed towards the identification of the recombination centers involved in the TL process, with the glow curves presenting several overlapping bands. TL spectroscopy measurements showed TL signal to be originated mostly from Cr3+ impurities. The stability of TL signal storage (fading) was evaluated.
This material is based upon work supported by the National Science Foundation under Grant No. 1653016.

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I3D.2 Wide band gap nanoparticle thin films as photoconductive sensors of high-energy radiation

Dr. Marilou Raduban[1,2], Mr. Tomoki Kato[3], Mr. Yusuke Horiuchi[3], Assoc. Prof. Shingo Ono[3], Dr. Kohei Yamanoi[2], Dr. Michal Kohout[4], Dr. Jiří Olejníček[4]

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Vacuum ultraviolet (VUV) radiation that spans the wavelength range from 200 nm down to 100 nm is indispensable in numerous technological applications, such as surface treatment, photochemical processing, optical cleaning of semiconductor substrates, and sterilisation of medical apparatus. It is also important for scientific research, primarily in gas chromatography and molecular spectroscopy. 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, to match the rapid progress. This talk presents our work in harnessing the wide band gap of titanium dioxide (TiO_2) along with its excellent physical, chemical and optical properties to demonstrate the potential of nanoparticle TiO_2 thin films as photoconductive sensors of VUV radiation. The crystallinity, optical quality, band gap energy, and crystallite size of the films can be controlled by manipulating the film's thickness and type of substrate, correspondingly affecting the sensor's photoresponsivity [1]. Post-fabrication treatment with gamma-ray irradiation leads to the creation of oxygen defects, but subsequent recovery of these defects enhances the sensor's photoconductivity [2]. Initial results on the coupling of the nanoparticle thin film sensor with scintillators that detect a wider range of radiation beyond VUV (like charged particles, neutrons, gamma rays) will also be discussed. Development of the TiO_2 thin film sensor is expected to contribute to the enhancement of the use of VUV radiation in an increasing number of important technological and scientific applications.

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I3D.3 Identification of single optically addressable spins in a two-dimensional material.

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Optically addressable spins in materials are important platforms for quantum technologies, such as repeaters for quantum networks [1]. Identification of such systems in two-dimensional (2D) layered materials offers advantages over their bulk counterparts, as their reduced dimensionality enables more feasible on-chip integration into devices. In this talk I will introduce a two-dimensional material that hosts bright single photon emitting defects: hexagonal Boron Nitride (hBN). I will show my recent results of room-temperature optically detected magnetic resonance (ODMR) from single atomic defects in hBN [2]. These results represent the first identification of room-temperature ODMR for single defects in a van der Waals material and offers a promising route towards realising a room-temperature spin-photon interface for future quantum technologies.

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3D.1 Deep Blue-Emissive Molecules With Combined Hot Exciton and Aggregation-induced emission (AIE) Features as Efficient Emitters for Non-Doped OLEDs

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In this work, two blue emissive molecules, namely PPI-DPB-TPA and PPI-DPB-PhC, with a combined feature of hot exciton and aggregation-induced emission (AIE) are designed to improve the performance of deep blue organic light-emitting diodes (OLEDs). The hot exciton process will increase the internal quantum efficiency via a reverse intersystem crossing of high-lying triplet states to singlet states (Sm ↔ Tn; m ≥ 1, n ≥ 2) while the AIE property will enhance the luminescence in the solid state. PPI-DPB-TPA and PPI-DPB-PhC comprised a diphenylbenzene (DPB) as a core substituted with 1-phenyl-1H-phenanthro[9,10-d]imidazole (PPI) as an acceptor (A) and triphenylamine (TPA)/phenyl carbazole (PhC) as a donor (D), respectively, formulating D-π-A blue emissive fluorophore are successfully synthesized and characterized. The photo-physical, thermal, and electrochemical results, and theoretical calculations reveal that both molecules exhibit combined hot exciton and AIE characteristics and intense blue color emission with high photoluminescence quantum yields of 79% in the solid-state, high thermal and electrochemical stabilities. They are successfully fabricated as a non-doped emitter in OLEDs. In particular, the non-doped device employing PPI-DPB-PhC as an emissive layer (ITO/HATCN (6 nm)/NPB(30 nm)/TCTA (10 nm)/PPI-DPB-PhC (30 nm)/TPBi (40 nm)/LiF (1 nm)/Al (100 nm)) shows excellent electroluminescence (EL) performance with a narrowband deep blue emission, a low turn-on voltage of 2.6 V, and maximum external quantum efficiency (EQEmax) of >6.4%.

3D.2 Optical Gain Spectroscopy of Nanostructured Materials: Bigger is Better

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Nanostructured semiconductors dominate opto-electronics to date, mainly in the framework of quantum wells and dots grown by vacuum epitaxial methods. A next (r)evolution in this field is happening as we speak ,through the use of solution processable nanostructured materials. Indeed, by combining low temperature, substrate independent processsing with size-tunable optical properties, such as luminescence and optical amplification (gain), these 'nanocrystals' are excellent building blocks to realize small footprint LEDs and lasers.

In this talk, I will overview our efforts towards integrated laser sources based on colloidal inorganic nanomaterials, quantum dots (QDs), in short. To do so, we will start out with discussing how optical gain, a premise to build lasers, is measured and quantified in these unique materials. Building on this framework, I will explain how net stimulated emission develops in several nanoscale architectures, from 0D to 2D systems, and how we reached after nearly a decade of research a set of materials with excellent gain metrics on all fronts. Finally, I will show a few results of combining these flexible materials with integrated photonic cavities, thereby realizing ultra-small footprint lasers and unique on-chip coupled lasing systems.

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3D.3 Triplet-Triplet Annihilation: Magnetic Field Effects in Solution

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In triplet-triplet annihilation (TTA) the molecular energy of two photons is pooled and emitted as fluorescence of a single photon of higher energy. TTA is a promising means of accessing solar irradiance below the silicon bandgap and surpassing the Shockley-Queisser limit. In addition, TTA allows the output light wavelength to be tailored to a specific application via choice of molecule and functionalisation.

As TTA is a spin-selective process it exhibits a magnetic field response, which has traditionally been described and modelled in the context of Atkins & Evans' Theory (1). Here, we revisit the theory, motivating the origin of key equations and evaluating the assumptions behind them. We rederive the theory with an alternative choice of initial and equilibrium states which better captures the typical situation for TTA in solution. In doing so we also compute the relative contributions of all spin channels, not just the singlet channel. These new conditions fundamentally change the evolution of decoherence in the system, and thus the final magnetic field response equations. The ramifications of these updates are discussed in light of recent experimental results (2).

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3D.4 Optical Fiber Sensors in Tokamak Fusion Reactors

Mr Fernando Solis Fernandez[1], Dr Bart Ludbrook[1], Dr Shahna Haneef[1], Mr Mike Davies[1], Dr Xiyong Huang, Dr Dominic Moseley[1], Professor Rodney Badcock[1]
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3D | Optical materials 2, Downer, February 8, 2023, 1:15 PM - 3:30 PM

Nuclear fusion energy is a promising candidate to become a reliable clean source of energy. Tokamak fusion reactors utilise superconducting magnets that need to operate in cryogenic conditions. In such environments with high radiation levels, low temperature and EM noise, classic voltage-based sensors are unreliable and optical fiber sensors (OFS) may prove to be an effective alternative. However despite the tolerance of optical fibers to EM noise, radiation created in these kind of reactors can cause an excessive attenuation in the fiber, known as radiation-induced attenuation (RIA), that renders them unusable.

Although RIA has been widely studied [1], there is still much to be discovered about it in extreme environments. The purpose of our research is to learn about the RIA characteristic profile in the operation conditions of Tokamak reactors as well as investigate the use of light to mitigate radiation damage (photobleaching). Specifically, we look at wavelength and power dependence of photobleaching effectiveness and wavelength dependence of the RIA at low temperatures to better understand what radiation-induced defects are the most relevant and how to mitigate them

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I3E.1 Phase tools for synthetic biology: shaping condensate dynamics with ATP:Mg2+

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3E | Bio 4 – responsive and biological materials, Sigma, February 8, 2023, 1:15 PM - 3:30 PM

Can we use biomolecular condensates as tools to trap RNA? Here, salt concentrations were used to alter the biophysical properties of nature-inspired phase-separated compartments, which not only gives insights into biological phenomena, but also provides an innovative method for localising RNAs.

The nucleolus is a phase separated compartment formed during interphase in eukaryotes as the site of ribosome biogenesis. Nucleoli have slow viscoelastic condensate dynamics that are currently not well captured by in vitro models. We show that an interplay between magnesium ions (Mg2+) and ATP ultimately shapes both the dynamics and the physical state of an in vitro nucleolus model of nucleophosmin 1 (NPM1) protein and ribosomal RNA (rRNA). At high free Mg2+ concentrations, rRNA is fully arrested and the condensates are gels. Using quantitative fluorescence microscopy, we show that the NPM1-rRNA droplets can 'age' and that RNA compaction is temperature-reversible, indicating that base paring contributes to the slowed RNA dynamics. The dynamic arrest of RNA can be reversed by ATP, resulting in complete liquefaction of previous gel-like structures. Within cells, ATP levels are controlled by biomolecular reactions, and we demonstrate that a dissipative enzymatic reaction can similarly control the biophysical properties of in vitro condensates through depletion of ATP. Our results not only illustrate how cells could regulate the dynamics of RNA-based condensates, such as the nucleolus, but also provide a step towards control of processes crucial for bottom-up synthetic biology.

I3E.2 See the Light: Advanced Light Activated Materials for 3D Bioprinting & Regenerative Medicine

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3E | Bio 4 – responsive and biological materials, Sigma, February 8, 2023, 1:15 PM - 3:30 PM

Biofabrication technologies, including 3D bioprinting and 3D bioassembly, enable the generation of engineered constructs that replicate the complex 3D organization of native tissues via automated hierarchical placement of cell-laden bioinks, tissue spheroids, and/or bioactive factors (1,4]. Radical polymerization combining light and photo-initiators to generate radicals for crosslinking photo-polymerizable macromers, has been widely employed in 3D bioprinting of cell-laden hydrogels. Recent developments have now resulted in the availability of a plethora of bioinks, new printing approaches, and technological advancement of established techniques. Despite rapid advances, no universal bioink exists and a major bottleneck lies in designing hydrogel bioinks that are both cell-instructive and compatible with high resolution 3D-biofabrication techniques. This requires optimization of bioinks for each individual biofabrication technique and tissue type.

This study describes the development of a novel platform visible light photoinitiator system for gelatin-based bioinks using ruthenium (Ru)/sodium persulfate (SPS) (Vis + Ru/SPS) that crosslinks in the visible light range (400-450nm), exhibiting increased cell viability, metabolic activity, shape fidelity and penetration depth compared to traditional ultraviolet (UV) crosslinking that is more damaging to cells.

Furthermore, we demonstrate for the first time that versatile photo-clickable thiol-ene based hydrogels based on allylated gelatin (GelAGE) and gelatin-norbonene (GelNOR) combined with Vis + Ru/SPS have unique physico-chemical and rheological properties of a universal bio-ink, and are successfully able to be printed across multiple biofabrication technologies, including extrusion-based bioprinting, high resolution lithography-based (DLP) bioprinting and microfluidics platforms [1,4,7,8].

Importantly, tailoring macromolecular chemistry offered by the platform by varying photoinitiator and thiolated crosslinker (DTT, PEG-SH) concentration, we modulated the cell-instructive tissue niche for multiple cell types via covalent incorporation of thiolated bioactives (e.g. heparinSH), nanocomposites (e.g. strontium, Laponite) and tailored mechanical stiffness of cell-laden bioinks, yielding enhanced chondrogenic and osteogenic differentiation and vascular network formation [2,3,5,9].

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I3E.3 Design and synthesis of 'smart', self-assembling molecular subunits with DNA origami

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3E | Bio 4 – responsive and biological materials, Sigma, February 8, 2023, 1:15 PM - 3:30 PM

DNA can be used as a building material for the self-assembly of well-defined 3D molecular structures and dynamic machines, with well-defined chemical properties. Such DNA nanostructures can be harnessed as 3D breadboards to control the spatial localisation of nanoparticles or biomolecules at resolutions well below 10 nm or to explore novel principles in nanoscale construction. In this presentation, I will discuss the theory and design of 'smart' bio-inspired molecular subunits, that we embody experimentally with DNA origami subunits. In one instance, we demonstrate how geometric frustration can be used to encode the global geometry of polymers in subunits that are only capable of myopic interactions with their neighbours1. In another, we design and synthesis DNA origami subunits that can bind stably with molecular cargo, yet simultaneously and rapidly exchange their cargo when required2, thus mimicking behaviours observed in complex biomolecular machines such as the DNA replisome. Both examples provide new molecular design principles that may be used for innovative nanoscale construction.

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3E.1 Toxicity and selectivity studies of linear lipopeptide battacin analogues using model membrane

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3E | Bio 4 – responsive and biological materials, Sigma, February 8, 2023, 1:15 PM - 3:30 PM

The current findings on the mechanism of action of linear lipopeptide battacin still could not explain the toxicity or the selectivity of the analogs [1, 2]. The purpose of this work is to elucidate the lipopeptides' selectivity over the gram-negative bacterial and mammalian membranes. This knowledge is useful in designing a new antimicrobial lipopeptide effectively.

Specifically, the linear lipopeptides with varying fatty acid chains interacted with different combinations of phospholipids to mimic the inner membrane of gram-negative bacteria and the composition of the mammalian membrane. The peptide-membrane interaction was analyzed by electrical impedance spectroscopy (EIS), small-angle scattering (SANS), and all-atom molecular dynamic (MD) simulation.

We found that cholesterol reduced the peptide-membrane interaction of all analogs. To explore the role of cholesterol, we tested these peptides against cylindrical and negative curvature lipids in the absence of cholesterol. The peptide-membrane interaction of the shorter fatty acid chain lipopeptide (C6B) was also significantly reduced when interacting with cylindrical lipid in comparison to the longer chain analog (C13). This implies that the type of lipids influences the selectivity of the analogs.

We also showed that the fatty acid chain length affects the aggregation formation of peptides on the membrane. Only C13 peptide could aggregate through the fatty acid chain on the membrane and this arrangement resulted in greater membrane perturbation. We hypothesized that the self-associated form of C13 lipopeptide altered the topology of the peptide and its binding strength, which causes the peptide to be active on all types of phospholipids.

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3E.2 Exosome inspired RNA compartmentalisation in complex systems

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3E | Bio 4 – responsive and biological materials, Sigma, February 8, 2023, 1:15 PM - 3:30 PM

The mimicking of biological communication and information transfer in artificial multicellular systems has been a target for researchers over the past few years. Development of artificial protocell systems has the potential to increase our understanding of cellular processes and biological functions, produce therapeutic technologies for advancement of global healthcare, and give rise to further understanding into how life evolved on earth.

Progress towards replicating these complex biological pathways in synthetic systems has only recently come to fruition. A variety of compartmentalised protocells have been fabricated with lipid vesicles, polymersomes, complex coacervates, and hydrogel microparticles. While signalling usually involves diffusion of small molecules from sender protocells to receiver protocells, to activate compartmentalised enzyme cascade reactions,[1] recently, this diffusion-based signalling has been expanded to include naked nucleic acids, which is a significant step towards more life-like information processing in synthetic cells.[2] However, in nature, transfer of genetic information between cell populations occurs with nucleic acids protected in further subcellular compartments – exosomes, as was demonstrated in 2007 for the first time for RNA communication between cells.[3]

Coacervate protocells have been successfully formed, along with light responsive charge switching polymersomes. Encapsulation of RNA into the polymersomes was successful, as was loading of polymersomes into coacervates. This example of UV triggered nucleic acid containing polymersome transfer between coacervates and living cells is a proof of concept for going beyond more stable DNA-based transfer.

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3E.3 Structural Characterisation of Silk Fibroin Based Hydrogels Using Small and Ultra-Small Angle Neutron Scattering Techniques.

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3E | Bio 4 – responsive and biological materials, Sigma, February 8, 2023, 1:15 PM - 3:30 PM

Hydrogels made of proteins are hierarchical three-dimensional structures. These are formed either by physical or chemical cross-linking of protein molecules in solutions. Their network structure can retain large amount of water. Various natural form of proteins such as silk fibroin, resilin, gelatine, collagen etc, are commonly used to make protein based hydrogels. These hydrogels are gaining significant interest in biomedical field especially in the field of tissue engineering and regenerative medicine. However, engineering specific hydrogels from protein alone has its own limitations (e.g. poor mechanical properties).

Tailoring these hydrogels by introducing other molecules within the structure may provide answers to many such limitations. Our group is pioneer in hydrogel fabrications (especially from silk fibroin) and their characterisation. Silk fibroin has been widely recognized as a promising biomaterial because of its excellent biocompatibility, high mechanical strength, ability to support cellular interactions, biodegradability, and abundant availability in nature. We have employed small and ultra-small angle neutron scattering (SANS, USANS) to characterise nano and microstructure of various hydrogels. These techniques have been exceptionally useful for studying complex materials of industrial importance in recent years. SANS and USANS are well-established for characterisation at the 1 nm to 20 µm length scales, are mostly non-destructive, and particularly useful to study systems, in-situ, and within complex sample environments. In this work we report nano and microstructures of several hybrid composite hydrogels of silk fibroin.

Knowledge gain through SANS and USANS about the structures, provided us tools to enhance the biochemical and physicochemical properties these composite hydrogels for certain applications. It also provides valuable understanding to corelate properties of molecular building blocks to the microscopic length scale of samples.

3E.4 Controlled Spatial Fabrication of Metalloprotein Nanostructures for Bio-Interfacing

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3E | Bio 4 – responsive and biological materials, Sigma, February 8, 2023, 1:15 PM - 3:30 PM

A variety of biomaterials have been developed using the natural capacity of self-assembling proteins to polymerize into highly structured filaments for application as scaffolds to align functional molecules. For bioelectronic applications, protein scaffolds can be engineered to function as electronically conductive nanowires, which may be further functionalized with active sites, such as redox molecules and enzymes.[1,2] In this way, integration of biological systems with electronic devices may be revolutionized by using proteins that have tunable electronic properties.[1,3]

Here, we harnessed a modular protein engineering platform to build metalloproteins nanowires with unique charge transfer behaviors for the interfacing of electronic devices and biological systems. We used an ultrastable filamentous protein called gamma-prefoldin (γPFD) from Methanocaldococcus jannaschii as scaffold to align conductive domains and obtain electronically conductive metalloprotein nanowires.[2] A variety of metalloproteins were aligned along the longitudinal axis of protein filaments, to functionalize the filament in an ordered and controlled manner. Metalloprotein nanowires comprised of γPFD and either cytochrome c3 or rubredoxin metalloproteins were shown to be highly conductive by potentiometric techniques and conductive AFM of single nanowires. In addition to assembly into linear nanowires, our metalloprotein nanowires are building blocks that could be used to construct conductive nanostructures in bioelectronic devices or interface with functional materials.

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K.11 Guiding Peptide-driven Exfoliation and Organization of 2D Nanomaterials

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Keynote Session 11, Bay Trust Forum, February 8, 2023, 4:00 PM - 4:40 PM

Peptides provide a versatile platform for the generation and organization of nanomaterials in liquid water. However, their application and use on two dimensional (2D) nanosheet structures such as graphene, h-BN and MoS2 is hampered due to a lack of fundamental data regarding the structure/function relationships of these bio-nano interfaces. Together with experimental characterization, molecular simulations can provide complementary insights into these challenging interfaces.1-3 Here, our strategy uses bioconjugate hybrids of peptides and fatty acids to exfoliate materials into 2D nanosheets in aqueous media. The role of molecular simulations in revealing the molecular scale characteristics of the peptide-driven exfoliation process are discussed for graphene, particularly in the role of the fatty acids in potentially reducing defects in the exfoliated material.3,4 Umbrella sampling simulations are also used to provide unprecedented insights into both the peptide-driven exfoliation and suspension mechanisms.5 Key to our progress here are advancements in our simulation strategy to model peptide/h-BN and peptide/MoS2 interfaces. This required development of interfacial force-fields for describing bio-interactions at h-BN and MoS2 nanosheet6 interfaces in aqueous media, based on first-principles calculations. Replica-exchange with solute tempering molecular dynamics simulations are used to explore the contact between the peptides and the nanosheets, to guide the design of effective bioconjugates for exfoliation and assembly. The outcomes of our simulations provide a strong foundation for future work to design7 and deploy these molecular bioconjugates in the self-assembly of 2D heterostructures.

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K.12 New mechanism in memristors revealed – prospective and challenges

Mr Shaochuan Chen[2], Mr Zhen Yang[3], Prof Yuchao Yang[3], Dr. Ilia Valov[1,2]
[1]Research Centre Juleich, Juelich, Germany, [2]RWTH-Aachen University, Aachen, Germany, [3]Peking University, Peking, China

Keynote Session 12, Skellerup & WSP, February 8, 2023, 4:00 PM - 4:40 PM

Properties, functionalities and stability of memristive devices are determined by three main factors – materials, physical processes and operation scheme, where the first two factors are inherently related. It is a priority of the ongoing research to improve memristors in several important aspects including multi-functional use, variability, state stability and degenerative processes. A way to success is to attain deep understanding and control over the physical processes involved in the formation of different resistive states and based on this knowledge to design reliable materials system being with predictable and adjustable properties. Several important aspects of the operation principles have been relieved, such as effects of protons and ambient moisture, interface interactions, migration of cations believed to be immobile, nanobattery effect, influence of the capping layers and film thicknesses etc.

In this work, we present a new mechanism observed in oxide memristors allowing for significant improvement of the device characteristics and stability. The switching performance depends on one hand side on the materials used for electrodes, their electrochemical activity and redox potential. On the other hand side it depends on the polarity of forming and operating the memristor. Our devices are able to operate (formation and switching) in both polarities however, the characteristics are not the same. The in situ TEM analysis have shown that contribution of different ionic species is responsible for two distinctive switching mechanisms that in turn determine the performance. Based on this knowledge we were able to design devices showing multiple functionalities and with significantly improved characteristics.

Pl.03 Academic Entrepreneurship – Selling Out or Delivering Value?

M. Cather Simpson[1]
[1]*University of Auckland,*

Plenary Session 3, Bay Trust Forum, February 8, 2023, 4:45 PM - 5:35 PM

Today's universities increasingly are tasked with achieving positive economic, social and environmental impact upon their cities, regions, countries and globally through positive return on R&D investment, a concept adapted from the business world. One way to create value from research funding is to spin technology out of the university lab and into the marketplace. Is that what universities should be doing?

Research commercialisation steps well outside of the traditional academic mandate to teach the next generation and to create new knowledge through novel, curiosity-driven research. In this talk, I will explore this rise of the academic entrepreneur, with particular emphasis upon what it means for the ivory tower, the technology landscape, and whether this is an activity that universities, research institutes, centres of research excellence and the like should undertake.

Pl.04 Semiconductor Nanostructures for Optoelectronics Applications

Chennupati Jagadish[1]
[1]*The Australian National University, Australia*

Plenary Session 4, Bay Trust Forum, February 9, 2023, 8:30 AM - 9:20 AM

Semiconductors have played an important role in the development of information and communications technology, solar cells, solid state lighting. Nanowires are considered as building blocks for the next generation electronics and optoelectronics. In this talk, I will present the results on growth of nanowires, nanomembranes and microrings and their optical properties. Then I will discuss theoretical design and experimental results on optoelectronic devices. In particular I will discuss nanowire and micro-ring lasers and integration of nanowires and microrings. I will also present the results on polarization sensitive, broad bandwidth THz detectors operating at room temperature. Nanowire based energy devices such as solar cells and photoelectrochemical (PEC) water splitting will be discussed. I will discuss about Neuro-electrodes to study brain signaling to understand dementia. Future prospects of the semiconductor nanostructures will be discussed.

K.13 Conductive Dithiolene-Based Metal-Organic Frameworks for Electrocatalytic H2 Production

Prof. Smaranda Marinescu[1]
[1]*University of Southern California, Los Angeles, United States*

Keynote Session 13, Bay Trust Forum, February 9, 2023, 9:25 AM - 10:05 AM

Sustainable hydrogen evolution reaction (HER) from water has emerged as a promising pathway for the storage and conversion of solar energy in chemical bonds. Hydrogen is a valuable energy carrier that can be transformed into electricity using fuel cell technology or used in the production of industrially relevant chemicals such as ammonia and methanol. Heterogenization of molecular catalysts is an attractive strategy to combine the advantageous properties of homogeneous and heterogeneous catalysis. Metal-organic frameworks (MOFs) have emerged as a promising class of materials; however, their insulating nature has limited their applications in electronics and electrocatalysis. We have demonstrated the successful integration of metal dithiolene units into one and two-dimensional frameworks by using dinucleating and trinucleating thiolate-based ligand scaffolds. The developed metal dithiolene frameworks display high activity for the electrocatalytic HER in acidic aqueous media. The HER performance of the MOF-based electrocatalysts is investigated, to understand the charge transfer properties of the constructed MOF/electrode architecture. Density functional theory calculations were applied to understand the structure of the MOF and its mechanistic pathways for the HER. We expect the design principles discovered in these studies to have a profound impact towards the development of advanced materials and sustainable technologies.

K.14 Dynamic protein coatings modulate nanomaterials interactions in the context of nanotoxicology and nanomedicine

Professor Duncan Sutherland[1]
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Keynote Session 14, Skellerup & WSP, February 9, 2023, 9:25 AM - 10:05 AM

Engineering nanomaterials are increasing present in our surroundings and in direct contact with living systems. Many application focus on use in life science applications aimed at drug delivery, bioimaging contrast agents or as tools for research, far more applications are not intended for medical use, but release of nanoparticles can lead to unintended exposure with the potential for nanotoxicity. The role of non-specific interactions of proteins and other biomolecules with nanomaterials leads to the formation of biomolecular coatings of host proteins which allow for specific interactions of these hybrid nanomaterials with the host [1]. There have been significant efforts to understand the formation and interactions of these biomolecular coatings with the aim to provide better predictive tools for potential toxicity of new nanomaterials. A significant challenge has been the dynamic nature of the interfacial interactions of proteins/biomolecule with the material with studies focusing on the long-lived strongly-attached fraction of the protein corona. Work in understanding strong and weak interactions of proteins at nanoparticles in the context of nanotoxicology will be presented. Including the importance of the host species and host sex in the formed corona with relevance for econanotoxicology testing [2,3,4]. We have quantified the fraction of weakly attached proteins and established a role for them in toxicity and biotransformation of silver nanomaterials [5,6]. In a last study, we devloped approaches to identify the weakly attached proteins and established a role for these proteins in modulating cellular association through non-specific interactions.

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K.15 The photoprotection mechanism in the black-brown pigment eumelanin

Professor Justin Hodgkiss[1]
[1]*Macdiarmid Institute of Advanced Materials and Nanotechnology, New Zealand*

Keynote Session 15, Bay Trust Forum, February 9, 2023, 10:05 AM - 10:45 AM

The natural black-brown pigment eumelanin protects humans from high energy ultraviolet photons by absorbing and rapidly dissipating their energy before proteins and DNA are damaged. The extremely weak fluorescence of eumelanin points towards non-radiative relaxation on the timescale of picoseconds or shorter. However, the extreme chemical and physical complexity of eumelanin masks its photoprotection mechanism. We sought to determine the electronic and structural relaxation pathways in eumelanin using three complementary ultrafast optical spectroscopy methods –fluorescence, transient absorption, and stimulated Raman spectroscopies. We show that photoexcitation of chromophores across the UV-visible spectrum rapidly generates a distribution of visible excitation energies via ultrafast internal conversion among neighboring coupled chromophores, and then all these excitations relax on a timescale of ~4 ps without transferring their energy to other chromophores. Moreover, these picosecond dynamics are shared by the monomeric building block, 5,6-dihydroxyindole-2-carboxylic acid. Through a series of solvent and pH-dependent measurements complemented by quantum chemical modelling, we show that these ultrafast dynamics are consistent with the partial excited state proton transfer from the hydroxy groups to the solvent. The use of this multi spectroscopic approach allows the minimal functional unit in eumelanin and the role of exciton coupling and excited state proton transfer to be determined, and ultimately revealed the mechanism of photoprotection in eumelanin. This knowledge has potential for use in the design of new soft optical components and organic sunscreens.

K.16 3D printed fluoropolymers: From Energy Harvesting to Microfiltration

Professor Amanda Ellis[1]
[1]*The University of Melbourne, School of Chemical and Biomedical Engineering, Parkville, Australia*

Keynote session 16, Skellerup & WSP, February 9, 2023, 10:05 AM - 10:45 AM

This talk highlights work on the 3D printing of fluoropolymers for applications as piezoelectric energy harvesters and novel porous membranes for microfiltration. The first part of the talk discusses piezoelectric fluoropolymers which convert mechanical energy to electricity, ideal for sustainably providing power to electronic devices. Eliminating electrical poling, via 3D printing with induced sheer, allows for the cheap, efficient production of piezoelectric polymers. Here, two-dimensional (2D) Ti3C2Tx MXene nanosheets with poly(vinylidene fluoride–co–trifluoroethylene) (PVDF-TrFE) are combined, leading to unprecedented fluoropolymer charge output without any electrical poling [1]. Molecular dynamic simulations show that strong electrostatic interactions at the interface of the two materials leads to a net polarisation in the PVDF-TrFE co-polymer, locked perpendicular to the Ti3C2Tx nanosheet basal plane. By electrostatically locking the net polarisation of fluoropolymers via nanomaterial templating, a new unforeseen fundamental mechanism is described, which can now lead to new levels of performance in piezoelectric technologies. This opens up a plethora of research opportunities to design piezoelectric composites with broad applicability, including in wearable energy harvesting, piezo-catalysis, piezo-photonics, and anisotropic sensors. The second part of the talk briefly discusses the hydrofluorination of poly(vinylidene difluoride) and its use as a flat sheet dPVDF microfiltration (MF) membrane prepared via direct ink writing (DIW), followed by non-solvent induced phase separation (NIPS) [2]. The fabricated dPVDF membranes show greater caustic resistance, as compared to the commercially available PVDF membranes with comparable fluxes. Further, fully integrated spacers provide optimum fluid dynamics to facilitate flow and reduce/delay fouling of these membranes [3].

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I4A.1 Melting in Extreme Environments Using Monte Carlo Simulations

Elke Pahl[1], Diana Yu[1], Gray Hunter[1]
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4A | Functional materials, 2D materials and ferroelectrics, Bay Trust Forum, February 9, 2023, 11:15 AM - 1:00 PM

We will present Monte Carlo melting simulations of atomic systems – nanoclusters and bulk materials - under extreme conditions and discuss new challenges introduced by huge pressures and strong magnetic fields. In order to describe melting we must sample in detail the atomic configurations that are accessible at temperatures spanning the melting transition. Additional complexity arises under extreme conditions, e.g., a homogeneous magnetic field breaks the symmetry as the orientation of individual atomic bonds with respect to the magnetic field direction matters. Restrictions to commonly used spherical or cubic boundary conditions are no longer adequate and the orientation dependence of the bonds prohibits the use of standard functional forms to fit potential energy surfaces. The use of machine-learning potentials will be explored that have the additional advantage of given access to energy gradients practically for free.

I4A.2 Functional van der Waals Materials: A New Avenue for Next-Generation Electronics

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4A | Functional materials, 2D materials and ferroelectrics, Bay Trust Forum, February 9, 2023, 11:15 AM - 1:00 PM

Metal thiophosphates[1] are a new 2D materials class of interest which, in many ways, are the 2D equivalent of complex oxides as changes in composition, stacking, or pressure in turn lead to large changes in bandgap[2], magnetic ordering temperature and type[1], ferroelectric ordering temperature[1,3], possible Kitaev physics[4] (i.e. quantum spin liquids) and even the appearance of superconductivity.[5] I shall present the materials characterization of CuInP2S6 and related self-assembled CuInP2S6/In4/3P2S6 heterostructures as a case study for this materials class in particular and 2D materials in general to show how the underlying physics is affected by chemical and structural modifications. When alloyed with excess In, the compound spontaneously forms self-assembled heterostructures as the material is cooled from a cation liquid state where mobile Cu and In cations exist within a rigid [P2S6]4- framework. Upon freezing, the disordered cation sublattice separates into two distinct phases, one of which is ferroelectric (CuInP2S6).

The presence of these self-assembled heterostructures imparts strain to the ferroelectric phase and increases its TC [3]. The functionality of the CuInP2S6 phase is determined by the details of the phase separation (i.e. nanoconfinement of the CuInP2S6 domains suppresses ferroic ordering)[6,7] which in turn is affected by temperature and pressure. I will also discuss recent efforts in materials characterization where our team determined that the heterostructured phase evinces a tunable quadruple potential well for the ferroelectric phase.[8] Finally, I will discuss recent experimental efforts on the 2D multiferroic CuCrP2S6 compound.[9]

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I4A.3 In-silico prediction of functional on-surface supramolecular materials

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4A | Functional materials, 2D materials and ferroelectrics, Bay Trust Forum, February 9, 2023, 11:15 AM - 1:00 PM

Surface-adsorbed supramolecular assemblies are of enormous fundamental interest, however their impact beyond the laboratory has been limited for two reasons. The first reason stems from the molecular self-assembly process which builds these materials. This process is notoriously difficult to predict, making it difficult to design supramolecular materials for specific applications. The second reason is economic: large-scale production of supramolecular materials is costly, and the ability of these materials to compete with existing ones is questionable. In this presentation, I will summarise our efforts to develop a computational framework for predicting the outcome of molecular self-assembly processes on metallic surfaces [1 - 3]. This framework combines a gamut of techniques (density functional theory, machine learning, and Markov chain Monte Carlo) and predicts assemblies which are in good agreement with experimental data. Moreover, by applying this framework to the case of surface-adsorbed metal complex molecules, we can identify strategies to build supramolecular assemblies with novel magnetic properties [4]. Towards the end of this presentation, I will present our fledgling attempts to incorporate density functional theory calculations into microeconomic theory, as well as an application to predict market shares of platinum monolayer catalysts for hydrogen fuel cells [5].

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4A.1 Highly Processable Edge Functionalised Graphene: From Dough to Dispersions

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4A | Functional materials, 2D materials and ferroelectrics, Bay Trust Forum, February 9, 2023, 11:15 AM - 1:00 PM

Graphene, a nanocarbon with exceptional physical and electronic properties, has the potential to be utilised in a myriad of applications and devices. To realise this, the development of scalable chemistries is required that facilitates processing and fabrication in such a way that the inherent properties of graphene are maintained within the material structures or devices.[1] A range of chemical processes have been developed both in our laboratories,[2,3] and others for the production of graphene dispersions in both aqueous and organic solvents but these invariably produce dispersions of low concentration and limited processability. To overcome this, we have been able to selectively oxidise the edges of the graphene sheets in graphite in large scale (> 400 g per batch) that yields aqueous dispersions of edge functionalised graphene (EFG) nanoplatelets 200 times higher (100 mg mL-1) than for a typical chemically converted graphene dispersion.[4] In addition, EFG forms the first example of a graphene 'dough' with water that will take up a variety of other liquids including both hydrophobic and hydrophilic solvents, ionic liquids as well as polymer dispersions. This allows the creation of conductive, binder-free graphene doughs that have the potential for mouldable electrodes, polymer composite development, battery/supercapacitor anodes and many other applications. In this presentation, we will discuss the synthesis, characterisation, functionalization and properties of this remarkable new graphenic material as well as a range of applications that it is being used for.

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4A.2 A comprehensive first-principles investigation on the defect chemistry of high performance lead-free BZT-BCT ferroelectric material

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4A | Functional materials, 2D materials and ferroelectrics, Bay Trust Forum, February 9, 2023, 11:15 AM - 1:00 PM

Owing to the increased environmental and health concerns and corresponding legislation to substitute lead-based ferroelectric materials, there is an urgent need for high performance alternatives to Pb-based piezoelectric ceramics. BaTiO3-based piezoelectric ceramics are considered as one of the promising Pb-free substitutes [1,2]. Among them (1− x)Ba(Zr0.2Ti0.8)O3–x(Ba0.7Ca0.3)TiO3 (BZT–BCT) system with extraordinarily high piezoelectric properties (d33 > 600 pC/N) have aroused extensive attention [3].

Ferroelectric properties of BZT-BCT materials have been widely studied for their implementation in various applications such as energy harvesters, flexible sensors and energy storage capacitors [4,5,6].

Understanding native point defects is fundamental in order to comprehend the properties BZT-BCT materials in these technological applications. In my research work a computational approach that integrates ab initio electronic structure and thermodynamic calculations is used to determine point defect stability in BZT- BCT systems over a range of temperatures, oxygen partial pressures and stoichiometries.

Defect formation energies of oxygen, titanium, calcium and zinc vacancies are calculated. The resulting defect formation energies for all possible charge states are then used in thermodynamic calculations to predict the influence of temperature and oxygen partial pressure on the relative stabilities of the point defects.

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4A.3 Bio-Inspired Approaches Towards Graphene/h-BN Nanosheet Assembly Under Sustainable Conditions

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4A | Functional materials, 2D materials and ferroelectrics, Bay Trust Forum, February 9, 2023, 11:15 AM - 1:00 PM

Two dimensional nanosheet materials such as graphene and hexagonal boron nitride (h-BN) are poised to make major advances due to their transformational electronic properties. While individually these materials span the range of conductive (graphene) to insulating (h-BN) materials, the ability to drive the precise assembly of these nanosheets into heterostacks could prove to be important for a variety of applications including biosensing and energy harvesting/storage. Some advances in this assembly capability have been achieved; however, they typically require laborious, energy and time intensive processes that remain limited. As an alternative to these approaches, bio-inspired methods, based upon the organization of materials in nature, could be exploited to drive sustainable heterostack formation in water to identify and quantify the emergent properties from these scaffolds. To achieve this capability, we have exploited materials binding peptides, termed P1 and BP7, with affinity for graphene and h-BN, respectively. These two peptides were incorporated into a single synthetic construct, termed BEAM (biomolecular exfoliant and assembly motif), where regioselective binding of the target materials has been demonstrated at the specific domains. The BEAM subsequently demonstrated the ability to drive exfoliation of individual graphene flakes from bulk graphite, where the biomolecules were non-covalently adsorbed to the carbon surface, thus presenting moieties to solution to drive heterostack formation via binding at exposed peptide domains. Taken together, this research is highly promising to achieve graphene/h-BN heterostack formation, but could also be applied for the assembly of different compositions of materials where regioselective ligand binding to multiple disparate materials is required. Such assembly capabilities could be important for structures beyond nanosheets for applications in a wide variety of areas ranging from nanomedicine to quantum devices.

I4B.1 Synthesis of hierarchical metal nanostructures with high electrocatalytic surface areas

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4B | Catalysis and porous materials, Skellerup, February 9, 2023, 11:15 AM - 1:00 PM

Research in the field of 3D hierarchical structures is highly topical due to their highly porous nature that gives them wide-ranging and unique properties and applications. Processes exist for synthesizing 3D framework structures on the molecular level, such as metal-organic-frameworks and DNA-origami, or on the micron scale, such as metal foams and aerogels. 3D structures with dimensions on the nanoscale have remained elusive due to the challenging synthesis of materials with interconnected components that arrange in 3D. These 3D nanostructures are an exciting new class of material that bridge the gap between molecular and micron scales.[1]

In this presentation, I will present a synthetic concept for metallic nanostructures where i) the 3D material is built up from growth of nanoscale cores and branches in consecutive steps, ii) the metal components are connected by careful selection of metals with cubic and hexagonal crystal structures[2] and iii) the multi-step approach enables tuning of the reaction conditions during each step of the growth process to control the dimensions and 3D geometry of the nanostructures.[3]

I will demonstrate the importance these interconnected, 3D nanostructures by analyzing their electrocatalytic properties. The nanostructures have surface areas that are up to 100x greater that micron-scale foams, conductivity that matches state-of-the-art metal materials, and metal surfaces that can be chemically modified. By coating an oxygen evolution reaction (OER) catalyst nickel-iron oxyhydroxide (Ni/Fe-O(OH)) onto the surface of the 3D nanostructures, we show that these materials that make high performing electrocatalytic supports.

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I4B.2 Conversion of CH4 to high value chemicals by photocatalysis

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4B | Catalysis and porous materials, Skellerup, February 9, 2023, 11:15 AM - 1:00 PM

Methane conversion not only involves the environmental issue but also is related to high-value chemical production /clean energy supply, which has been attracting substantial interest over the last decades. However CH4 activation is energy intensive and kinetically very challenging so that methane activation is regarded as the “holy grail” in the catalytically chemical process. [1] Photocatalysis provides a cost efficient potential to activation of such small molecule under very mild conditions, while to achieve the potential is a huge challenge.[2]

Stimulated by our research outcomes on the charge dynamics in inorganic semiconductor photocatalysis, which reveal that the low reaction efficiency is due to both fast charge recombination and large bandgap of an inorganic semiconductor [3,4], together with the recent findings on atomic catalysis [5], we developed novel material strategies for photocatalytic methane conversion to methanol.

Highly dispersed atomic level iron species immobilised on a TiO2 photocatalyst show an excellent activity for methane conversion, resulting into ~97% selectivity towards alcohols operated under ambient conditions by a one-step chemical process [6]. Such photocatalyst is also very stable, promising an attractive industrial process of methane upgrade. The dominating function of the iron species has also been investigated in detail. Furthermore, we designed a flow system for relatively efficient methane to C2, achieving the benchmark results in this area.[7] In addition, C1 oxygenates can also be produced with nearly 100% selectivity by Pd and oxygen vacancy modified In2O3.[8]

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I4B.3 What makes Ruthenium Dioxide a benchmark electrocatalyst for the water splitting reaction? Root causes from a condensed-matter physics perspective

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The electrocatalytic efficiency of ruthenium dioxide (RuO_2) for the oxygen evolution reaction has made this material a subject of intense fundamental and industrial interest. The functionality of RuO_2 is rooted in its electronic and magnetic properties, determined by a complex interplay of lattice-, spin-rotational, and time-reversal symmetries, as well as the competition between Coulomb and kinetic energies. This interplay was predicted to produce a network of Dirac nodal lines (DNLs), where the valence and conduction bands touch along continuous lines in momentum space. We uncover, with unprecedented precision, experimental evidence for three DNLs using angle-resolved photoemission spectroscopy. These DNLs give rise to a flat-band surface state that is readily tuned by the electrostatic environment, and that presents an intriguing platform for exotic correlation phenomena. Our findings support high spin-Hall conductivity and bulk magnetism in RuO_2 and are likely related to its functional properties. This work signifies the first experimental evidence of Dirac physics in a material of genuine industrial relevance.

4B.1 Enhancing regeneration kinetics by tailoring the structure of the donor systems in organic dyes

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4B | Catalysis and porous materials, Skellerup, February 9, 2023, 11:15 AM - 1:00 PM

Controlling interfacial electron transfer (ET) between dyes attached to a semiconductor surface and redox mediators in solutions is crucial for increasing the efficiency of photo-electrochemical energy conversion. Studies focussing on the effect of molecular structure, particularly the exposure of the electrons located on the donor moieties are emerging, however clear design guidelines regarding the size and shape of donor moieties for enhanced electron transfer is lacking. This study focusses on the ET kinetics of 22 dye molecules with progressively larger donor units, both with single and double bond linker attachments to the same π-conjugated backbone. The ET kinetics were determined in the presence of two different redox mediators Co(bpy)3 and Co(Mebpy)3 using the transient absorption technique by monitoring the absorption of the dye cation radical decay. The measured rates are analysed using classical Marcus theory covering electrochemical driving force ranging between 0.1 to 0.88 eV. Donor units with increased exposed area show 4 to 6 times enhancement in ET rates compared to smaller donor units at the same driving force. The correlations in enhancement of ET rate as compared to the predicted Marcus rate is correlated with the outputs of quantum chemical calculations such as polarizability, dipole moment, COMO-RS volume and area will be discussed. Detailed study on different sized donor units with increasing driving force provides a fundamental understanding in creating new redox active molecules with fast interfacial electron transfer at very low driving force, hence low voltage losses.

4B.2 Tuning alkane/alkene adsorption separation selectivity through acidic H-ZSM-5 zeolites

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Ethylene and propylene are prevalently known as important feedstocks in petrochemical industries with respective worldwide production capabilities of over 170 and 120 million tons in 2016 [1-2]. As the resulting products generally contain ethane and propane impurities, the mixture gases need to be purified prior to further manufacture of downstream products. However, energy-intensive cryogenic distillation is currently used to produce high-purity alkenes (≥ 99.9%) despite its harsh operating conditions (≥ 23 bar and ≤ 243 K) [1, 3-4]. Therefore, adsorption separation, which is more cost- and energy-efficient, has been applied as an alternative approach.

In this study, ZSM-5 zeolite with an approximate channel diameter of 0.55 nm is chosen for studying alkane and alkene adsorption as well as its potential in alkane/alkene separation. Among all physical and chemical features, Si/Al ratio, which plays a significant role in promoting alkene adsorption [4-8], is further examined. The adsorption equilibrium and kinetics of alkanes (ethane and propane) and alkenes (ethylene and propylene) together with their isosteric heat of adsorption and ideal adsorbed solution theory (IAST) are also thoroughly investigated.

In summary, this work demonstrates the significance of low Si/Al adsorbent in promoting ethylene chemisorption while hindering the permeation of the larger adsorptive molecules, i.e. C3 hydrocarbon molecules, resulting in much higher ethylene and propane uptake than those of ethane and propylene, respectively. This study presents an integration of adsorption equilibrium and kinetics to be further exploited for alkane/alkene separation e.g. selective ethane/ethylene and propane/propylene separation where energy use for regeneration can be minimized.

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4B.3 Pure and mixed gas adsorption kinetics of ethylene and ethane in Mordenite, Zeolite 13X and ZJU-74a.

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4B | Catalysis and porous materials, Skellerup, February 9, 2023, 11:15 AM - 1:00 PM

More than 200 million tonnes of ethylene and propylene are produced annually as raw materials for products essential to society. Their purification by cryogenic distillation accounts for 0.3% of global energy usage.[1] Separation by porous adsorbents (such as zeolites or MOFs) is an alternative to reduce the energy demand of this process.

Adsorbent materials can achieve separation through equilibrium selectivity (differences in affinity) or kinetic selectivity (differences in adsorption rate).[2] This presentation details fundamental adsorption kinetics measurements of pure and binary mixtures of ethylene and ethane on the porous adsorbents Mordenite, Zeolite 13X and ZJU-74a. These fundamental measurements aim to understand the adsorption kinetics to leverage their power in optimising adsorption processes. The results also serve to better understand what types of materials exhibit superior kinetic separation, with subsequent process modelling educating the types of kinetic selectivity that are most desirable.

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I4C.1 Topology and magnetism in Heusler alloy Co2MnGa – outstanding magnetoelectronic properties for physics and applications

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4C | Magnetism magnetoelectronics, WSP, February 9, 2023, 11:15 AM - 1:00 PM

To develop powerful and energy-efficient 21st century quantum electronic technologies, topology has become a major factor in finding materials that have the outstanding physical properties needed. Topology can be described as the study of shapes that can be deformed continuously into each other, and electronic states that are protected by their topology are proposed for ultra-low-energy devices, having dissipationless electronic currents. Combining topological electronic states with magnetism could allow for spin topotronic devices, that take advantage simultaneously of the magnetic and topological physics, and even bring the use of quantum electronic properties to room temperature. Several years ago it was predicted that Heusler alloy Co_2MnGa was one such magnetic topological material [1], confirmed soon after in bulk crystals [2]. However, to use the outstanding properties of this material in real devices requires thin films and patterned thin film structures.

In this presentation I will describe our successes in producing high quality thin films of Co_2MnGa that show the signatures of topological electronic states in several magnetotransport phenomena, such as new record values of anomalous Hall [3], anomalous Nernst [4], and recently, spin Hall [5] effects – all persisting to room temperature. I will outline the potential implications of the exceptional Weyl-boosted magnetotransport properties of Co_2MnGa for devices that rely on spin currents, thermo-spin conversion [6] and spin-orbit torques, and I will show some examples of potential applications that are beginning to appear.

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I4C.2 Towards spintronics functionalization of nitrides

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Since the family of nitrides has reached the status of the second most important semiconducting material-class after Si the prospect of spintronics functionalization of GaN have gained in significance. In this context we employ a strong coupling between piezoelectricity and magnetism [1], shown to exist in paramagnetic GaN doped only weakly with Mn [2].

Here, using the direct SQUID magnetometry, we demonstrate the piezo voltage-induced control of magnetization in ferromagnetic (Ga,Mn)N layers [3] documented at the low end of cryogenic temperatures. We observe a strong reduction of the width of the hysteresis curve (from about 120 to 10 Oe) and a non-reversible magnetization switching for magnetic fields close to the coercive field under the influence of external electric field. The experimental data are interpreted within the frame of the Landau-Lifshitz-Gilbert description of the precessional motion of magnetization adapted to (Ga,Mn)N by allowing for the electric field control of the magnitude of trigonal deformation along the wurtzite c axis of GaN. This in turn affects the effective magnetic field acting on Mn ions. We show that atomistic spin model properly describes the magnitude of the magnetoelectric signal and the electric field induced switching of the magnetization in such a random ferromagnet as (Ga,Mn)N, where the ferromagnetic state is realized in a percolation fashion. However, the electric field induced magnetization changes are found volatile in the sense that the material returns to its initial state upon removing the electric field or the magnetization switching is non-reversible within the current experimental scheme.

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I4C.3 Multiferroics beyond electric-field control of magnetism

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Magnetoelectric multiferroic materials, with their combined and coupled magnetism and ferroelectricity, are key components of new energy efficient device architectures that exploit electric-field control of magnetism. In addition, the unusual crystal chemistries required to engineer such magnetoelectric coupling lead to a diversity of initially unanticipated functionalities. I will discuss the fundamental physics behind these exotic behaviors, and show how they are enabling applications of multiferroics ranging from catalysts for water splitting, environmentally benign pigments, scaffolds for stimulating cell growth and even to answering fundamental questions regarding the origin of the universe.

4C.1 Switchable Magnetic Dots for Cryogenic MRAM

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Magnetic memory elements have been developed over the last several decades and we can now make elements that function at cryogenic temperatures. The developing technology is based on the rare-earth nitrides (LN, L chosen from the 14 rare-earth elements), which have a wide range of magnetic properties in their cryogenic ferromagnetic phase. Control of the magnetic properties required for the devices is enormously enhanced in solid solutions of two rare-earth nitrides ((L,L')N) [1, 2, 3]. We have previously shown non-volatile memory storage using tunnel junctions [4, 5]. Industry demands for low-impedance structures have opened up a project of making switchable magnetic dots for direct integration with superconducting Josephson junctions. I will present the growth and investigation of dots comprising of tri-layers of two matched ferromagnetic (L,L')N layers separated by a non-magnetic layer. One (L,L')N layer is chosen to have a fixed magnetic moment direction while the magnetic alignment of the other (L,L')N layer is easily switched to enhance or cancel the net magnetic moment. This means that the tri-layer's magnetic moment can be switched on and off. An adjacent Josephson junction senses the fringe magnetic field of the dot to form the data-reading operation. We have been able to reduce the magnetic dots to diameters in single digit microns, very close to the 1 micron size sought by our commercial partners.

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4C.2 Heusler Alloy-Based Magnetic tunnel Junctions with Perpendicular Easy Axis for Magnetoresistive Sensors

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Magnetic tunnel junctions (MTJs) are currently at the forefront of spintronics research because their large magnetoresistance (MR) and high sensitivity make them an attractive application prospect for magnetic memories and magnetic sensors [1]. MTJs with perpendicular magnetic anisotropy (PMA) are advantageous over in-plane devices due to their scalability, faster switching time and higher signal-to-noise ratio due to the enhanced uniaxial orientation [1].

Heusler compounds are one of the most promising candidates for MTJ electrodes because their half-metallic states can help achieve 100 % spin polarisation at room temperature, leading to an infinite magnetoresistance ratio. Furthermore, these materials have additional advantages, including high Curie temperature and long spin diffusion length [2]. Recently, our group has discovered Weyl semi-metal behaviours [3] and PMA [4] in Heusler-based Co2MnGa ultrathin films, making it a promising material for exploring spin-polarising devices.

In this work, we used Co2MnGa electrodes to obtain perpendicularly magnetised MTJ stacks. We used thin-film sputtering and photolithography to fabricate the devices. We optimised the devices by precisely varying the thickness of each Co2MnGa and MgO layer and annealing conditions. We used the magneto-optical Kerr effect (MOKE) microscopy for domain imaging and MR measurements of the multilayer stacks. The MTJ showed strong PMA, and we could identify two distinct magnetic steps in the field sweep curve corresponding to the switching direction of the two magnetic layers. The devices also showed high MR, demonstrating that Co2MnGa-based perpendicular MTJs are a strong candidate for the next generation of spintronic devices.

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4C.3 Magnetism, magneto-elasticity, and magnetostriction at 3D/2D and at interfaces

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Magnetostriction is a physical phenomenon in which the process of magnetization induces a change in shape or dimension of a magnetic material. Nowadays, materials with large magnetostriction are used in many electromagnetic microdevices as actuators and sensors. By contrast, magnetic materials with extremely low magnetostriction are required in applications such as for electric transformers. Magneto-elasticity - the change of the exchange interactions upon the various tensile or compressive loadings or an inverse as the external magnetic field can induces sample shape and lenght change. Similarly, this pheomena could be induced by lattice vibrations (phonons)[1].

In first part we present a methodology based on the Néel model to build a classical spin-lattice Hamiltonian for cubic crystals capable of describing magnetic properties induced by the spin-orbit coupling like magnetocrystalline anisotropy and anisotropic magnetostriction, as well as exchange magnetostriction. We derive theoretical expressions for the parametrization of the exchange integrals and Néel dipole and quadrupole terms that link them to the magnetic properties of the material. We apply this method to develop a spin-lattice model for BCC Fe and FCC Ni, and we show that it accurately reproduces the experimental elastic tensor, magnetocrystalline anisotropy under pressure, anisotropic magnetostrictive coefficients, volume magnetostriction, and saturation magnetization under pressure at zero temperature[2]. The many of the phenomena for various material were verified by the in-house developed codes[3-4].

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I4D.1 Neuromorphic properties of nanowire networks

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4D | Nanostructures & novel materials, neuromorphic devices and transistors, Downer, February 9, 2023, 11:15 AM - 1:00 PM

Bottom-up self-assembly of metallic nanowires produces a network of nanoscale memristive junctions with highly heterogeneous interconnectivity. This bears strong resemblance to the structure-function relationship between biological neural networks and their neurons and synapses. In Ag-based nanowire networks (NWNs), we found that neuro-synaptic functionality is emulated by threshold-driven, bipolar memristive switching, augmented by coupling to the network. We also found that the internal memristive dynamics of metal-core Ag-PVP NWNs differs from that of Ag2Se atomic switch NWNs, indicative of differences in the nanoscale electro-ionic transport mechanisms. Interestingly, however, these differences do not appear to affect the neuromorphic properties of their collective nonlinear dynamics, with neuronal-like spiking statistics observed in both types of NWNs. This suggests the potential of NWNs as a platform technology for next-generation brain-inspired electronic devices.

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I4D.2 Dendrites as Digital Triggers

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This paper presents the concept of dendrites formed via Laplacian instabilities in material systems as physical unclonable functions (PUFs) that can be used as digital triggers to connect items in supply chains and inventories to their digital identities in databases. These triggers must be (1) different for every instance of formation to give each item its own unique identifier or "fingerprint", (2) simple to evaluate so that they may be "read" quickly within the use environment, and (3) well preserved in the presence of noise. These requirements are readily met by dendrites formed by diffusion limited aggregation (DLA) in electrodeposition processes [1], or by Saffman-Taylor instability in viscous fluid/air interactions [2]. Such dendritic patterns are typically fractal in nature [3], which allows for determination of uniqueness [4]; information entropy can be high enough to allow unambiguous tagging of extremely large numbers of items, but the structural entropy is low so that error determination is achievable. Another advantage of the fractal nature of the structures is that the self-similar elements, in this case bifurcations, are readily handled by widely available feature recognition software. Centimeter-scale patterns are easily read using cell phone optics, which greatly simplifies the use of the technology. Light scattering from reflecting facets or particles in the dendrites ensures that they cannot be easily copied. The paper will cover the information theory and formation/manufacturing aspects of the technology and will demonstrate its use in various pilot applications.

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I4D.3 Anisotropic epitaxial stabilization of a low-symmetry ferroelectric with enhanced electromechanical response

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Piezoelectrics interconvert mechanical energy and electric charge and are widely used in actuators and sensors. The best performing materials are ferroelectrics at a morphotropic phase boundary, where several phases coexist. Switching between these phases by electric field produces a large electromechanical response. In ferroelectric $BiFeO_3$, strain can create a morphotropic-phase-boundary-like phase mixture and thus generate large electric-field-dependent strains [1]. However, this enhanced response occurs at localized, randomly positioned regions of the film.

Here, we use epitaxial strain and orientation engineering in tandem — "anisotropic epitaxy" — to craft a low-symmetry phase of BFO that acts as a structural bridge between the rhombohedral-like and tetragonal-like polymorphs. Interferometric displacement sensor (IDS) measurements reveal that this phase has an 2x enhanced piezoelectric coefficient compared with typical rhombohedral-like BFO. Band-excitation frequency response measurements and first-principles calculations suggest that this phase undergoes a transition to the tetragonal-like polymorph under electric field, generating a further enhanced piezoelectric response and field-induced reversible strains [2]. These results offer a route to engineer thin film piezoelectrics with improved functionalities, with broader perspectives for other functional oxides.

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4D.1 Behaviour of Ag-Ag2S-Ag Atomic Switch Networks with the Addition of a Carbon Nanotube Network Layer

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4D | Nanostructures & novel materials, neuromorphic devices and transistors, Downer, February 9, 2023, 11:15 AM - 1:00 PM

The emerging use of atomic switch networks for reservoir computing has exciting implications for the scaling-down of computer systems. The atomic switches in these networks operate in a similar way to synapses in a biological brain. Therefore, unlike a traditional computer design (the "Von Neumann architecture"), the processing and memory elements of these networks are not separate. This integrated arrangement removes the rate-limiting step created by the need to transfer information between elements, meaning much less space is needed for the same computing power [1-3].

The Ag-Ag_2S-Ag atomic switch network has been well-established by the UCLA Gimzewski group as a neuromorphic system suitable for use in reservoir computing. However, the established fabrication method for these memristive nanowire networks, electroless deposition, is relatively complex and difficult to reproduce [1,4-5]. Here, we outline a simpler, more cost-effective fabrication method. In this method, store-bought silver nanowires in solution are drop-cast onto a photolithographically patterned carbon nanotube network and then exposed to gaseous sulfur. By using a carbon nanotube network layer, we were able to obtain Ag-Ag2S-Ag atomic switch networks that exhibited consistent memristive behaviour, such as strong/hard switching and time-grouped switching behaviour.

We propose this is due to some combination of greater network connectivity and thermal stabilisation provided by the presence of carbon nanotubes.

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4D.2 Brain-like properties of percolating networks of nanoparticles

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4D | Nanostructures & novel materials, neuromorphic devices and transistors, Downer, February 9, 2023, 11:15 AM - 1:00 PM

Percolating networks of nanoparticles (PNNs) have recently attracted interest because of their potential to be used as novel neuromorphic (brain-like) computing systems [1]. In these systems, electrical input and output signals will couple to the recurrent electrical signals within the network that provide neuromorphic functionality [2]. This raises important questions as to whether practical electrode configurations and network geometries might influence the brain-like dynamics. We first use the concept of criticality [3] (which is itself a key characteristic of brain-like processing) to quantify the neuromorphic potential of the devices, and find that in most cases criticality, and therefore optimal information processing capability, is maintained. In particular we find that devices with multiple electrodes remain critical despite the concentration of current near the electrodes. We also find that broad network activity is maintained because current still flows through the entire network [4].

Another measure of neuromorphic potential is the reservoir computing (RC) performance. RC is a neuromorphic computing paradigm in which the non-linear dynamics and memory capacity of the network are exploited for information processing. A range of nanoscale devices and novel architectures have been explored for RC [5], but PNNs have yet to be employed as the reservoir. Here we examine the performance of PNNs in two benchmark tasks: tenth-order nonlinear auto-regressive moving average (NARMA10) time series prediction and memory capacity. We expand on the study of network size by investigating its effect on RC performance, as well as the related effect of the number of output electrodes.

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4D.3 Transfer-free n- and p-channel graphene field-effect transistors using graphene grown directly at 100 oC

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4D | Nanostructures & novel materials, neuromorphic devices and transistors, Downer, February 9, 2023, 11:15 AM - 1:00 PM

Graphene has been hailed as wonder materials for electronics due to its outstanding charge transport properties. However, its lack of an electronic bandgap has hindered its application to large-scale field-effect transistor (FET) circuits, thereby making bandgap opening a key priority. Further, the fabrication of graphene devices to date conventionally requires the transfer of graphene from its growth substrate to a target substrate, which introduces defects and negatively impacts the device performance. Overcoming these challenges, we demonstrate a transfer-free approach for the low-temperature growth (~100 °C) and in-situ doping of monolayer graphene, which enables FETs with cutting-edge performance and stability. With a focus on nitrogen-doped graphene, we realize n-channel FETs with an on-off ratio of ~2×10^8, a mobility of ~1,500 cm^2/V s, and a subthreshold swing of ~ 90 mV/dec. Such devices are highly reproducible and exhibit high wafer-scale uniformity and thermal and bias-stress stability. Further, our approach is highly versatile, for instance also allowing the fabrication of p-channel FETs with a mobility of ~470 cm^2/V s and an on-off ratio of 2×10^5. The scalability and versatility of this transfer-free approach for the fabrication of both n- and p-channel graphene FETs pave the way for high-performance graphene-based complementary circuits for next-generation electronics.

I4E.1 Dynamics at the interfaces & spontaneous motions in liquid-liquid and gas-liquid-solid systems

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4E | Soft and dynamic matter, Sigma, February 9, 2023, 11:15 AM - 1:00 PM

Knowing the behavior of molecules at the interfaces accelerates novel applications & materials for nanomedicine, energy, environmental technologies, catalysis, and food. As the observed phenomena scale down and involve contacting different matter/phases, interfacial phenomena start to dominate the bulk behavior. The interplay of surface chemistry and hydrodynamics results in spontaneous re-arrangements and transport of molecules and the dynamics at the interfaces determine larger behavior and some aspects will be demonstrated in this talk.

The dynamics of the spontaneous mass transfer from the energies of contacting interfaces will be presented in the context of liquid-liquid and gas-liquid-solid systems. First, merging process of drops and factors involved in the kinetics of coalescence will be shown in reactive and non-reactive system. It is observed that the surfactant-free drop intrudes into the surfactant-laden drop in the form of a penetrating jet and mixing patterns within the coalescing drops are due to the force imbalance caused by capillary pressure difference and surfactant-induced Marangoni stresses; the intensity of the convective bulk motion is also influenced by the viscosity of the outer phase.

Similarly, in the 3-phase system, the surface chemistry at the gas-liquid-solid interfaces dictates the capillary pressure driven flow in porous media or thin tubes. Furthermore, relative position of fine particles in respect to immiscible fluids interface will be shown to depend on the interfacial energies.

I4E.2 Amphiphilic Self-Assembly Structure and Dynamics in Ionic Liquids

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4E | Soft and dynamic matter, Sigma, February 9, 2023, 11:15 AM - 1:00 PM

The strong coulombic and H-bonding cohesive forces in ionic liquids (IL) that drives their inherent amphiphilic nanostructure makes them effective solvents for a wide range of organic solutes and enables them to support the self-assembly of synthetic surfactants and lipids into micelles, vesicles, lyotropic liquid crystals, and microemulsions.[1] Modulating liquid nanostructure through these intermolecular forces alters not only the preferred amphiphile self-assembly morphology into spheres, cylinders, bilayers and more exotic structures but also the dynamics of the resulting self-assemblies in surprising ways. Here we show using neutron spin-echo specrotroscopy and small angle scattering coupled to rheology how changing IL composition and nanostructure can be used to alter self-assembly structure and dynamics, affecting a range of physical properties.

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I4E.3 3D printing cellulose: the influence of process parameters on crystal alignment

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4E | Soft and dynamic matter, Sigma, February 9, 2023, 11:15 AM - 1:00 PM

Cellulose is a natural biopolymer that can be used in a wide range of applications, including composite reinforcement, food additive, membrane, orthopaedics materials, and sensors [1-3].

Recently, the growth of the 3D printing market, particularly in the biomedical area (e.g. tissue scaffolds) and specialty applications, has made cellulose a material of choice to investigate [4-6]. Studies reported that the directional printing and the shear thinning characteristic of the cellulose gels causes alignment of the nanocellulose enabling the manufacture of 3D solids with anisotropic properties that are retained after the gel is dried or cured [7, 8]. The ability to control the alignment of cellulose while 3D printing provides scope to introduce tailored anisotropic properties.

Our research investigates the mechanical behaviour, and physical properties of cellulose nanocrystals (CNC) dispersed in water, 3D printed and dried into a solid 3D structure. Parameters such as printing speed, nozzle diameter and drying temperature were studied. Synchrotron X-ray diffraction and scanning electron microscopy (SEM) were used to characterise the cellulose crystal alignment. We found that the printing parameters and drying processes influenced the agglomeration of the cellulose crystals. This offers opportunities to tailor the properties of 3D printed objects in pre-determined axis direction and create physical anisotropy that can be exploited in tandem with a tailored 3D structure.

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4E.1 Dynamics and Behaviour of Ultra-Small Gold Nanoparticles at Bio-Membranes – Combining Experiment with Simulation

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4E | Soft and dynamic matter, Sigma, February 9, 2023, 11:15 AM - 1:00 PM

Introduction: Nanomaterials - materials with nanoscale dimensions - are widely investigated, especially in many biological settings. This is due to their potential us as advanced nano-medicines and diagnostic technologies,[1-4] antimicrobials,[5] as cellular probes, and in cellular-imaging,[6] among other applications.[1, 4, 5, 7] The commonality between all applications is that they utilise the nanosized features of the material, specifically their departure from traditional bulk-like properties. In general, nanoparticle-based technologies must interact with, and often cross, a cellular membrane to be useful.

Aim: To combine advanced experimental and computation studies to study the interaction of ultra-small gold nanoparticles (AuNP) at a synthetic bio-membrane.

Methods: A combination of small-amplitude - atomic force microscopy (AM-AFM) and molecular dynamics (MD) simulations will be used to study the fundamental behaviour of the AuNPs at the bio-membrane-liquid interface. The system of interest is a model system consisting of a supported lipid bilayers (SLB) which act as an archetypal bio-membrane. The lipid used will be 1,2-di-(9Z-octadecenoyl)-sn-glycero-3-phosphocholine (DOPC) supported by muscovite (mica), an atomically smooth, phyllosilicate substrate.

Results: We investigate the behaviour (dynamics, adsorption, translocation, and physical interactions) of 5 nanometre AuNPs with a SLB. The precise mechanism by which the AuNPs adsorb to the bio-membrane was elucidated, revealing several interesting behaviours: 1) initial adsorption, 2) nanoparticle incorporation within the bilayer, and 3) two-dimensional (2D) translocations within the upper-leaflet of the DOPC bilayer.

Conclusion: These interactions are of broad scientific and medical interest because nanomaterials have recently become a viable method for manipulating matter at the cellular level, particularly for therapeutic and diagnostic applications.

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4E.2 Unusual Geometries Following Drop Impacts Using Advanced Materials

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4E | Soft and dynamic matter, Sigma, February 9, 2023, 11:15 AM - 1:00 PM

The study of liquid drop impacts involves an extremely wide and diverse range of experimental parameters – for example the size and velocity of the drop, the impact velocity and angle, and the geometric configuration (e.g. drop-drop or drop-object). When considering the narrower field of vertical drop impacts onto a flat solid surface there is still much to research [1], but the outcomes have some general similarities. These impacts produce a known range of outcomes (e.g. fragmented or deposited drops) and may spread, retract or even rebound from the surface. Azimuthal symmetry is typically broken only in a stochastic manner.

This presentation will discuss our research into three situations in which unusual material properties influence the outcome of a vertical drop impact onto a flat solid surface. The materials are (i) microfabricated pillar arrays, which can non-randomly break a spreading drop's azimuthal symmetry [2]; (ii) ferrofluids, which form characteristic instabilities near a simple bar magnet [3]; and (iii) drying non-Newtonian dairy product solutions, which spread and retract according to the nature of the drying process [4].

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4E.3 Topographical surface tension gradients for passive motion of water micro-droplets

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4E | Soft and dynamic matter, Sigma, February 9, 2023, 11:15 AM - 1:00 PM

Numerous industry applications and increasingly green technologies require effective water management on metals and their alloys, such as: condensation control to prevent erosion of steam turbine blades[1], condensation control in Heating, Ventilation and Air Conditioning (HVAC)[2], and prevention of drop impact erosion and icing on wind turbines[3]. The main issue is that metals are hydrophilic, having strong adhesion during liquid-solid interactions, and coatings are not applicable. But in nature, micro- and nano-structured surfaces like the pillar-wetting gradient of cicada wings may be found[4]. Some spider silk consists of knot-joint couplings providing a surface tension gradient for droplet transportation[5]. Such surface tension gradients can passively transport sub-millilitre droplets without requiring external forces, even gravity.

Inspired by these examples from the natural world, we have designed passive gradient surfaces[6] and produced them via a one-step industrial method, laser ablation[7]. Goniometric measurements clearly demonstrate that these surfaces can promote the spontaneous motion of certain-sized droplets, which is beneficial for providing drop-wise condensation over film-wise. Ion-beam implantation of inert helium does not modify the surface chemistry but influences the surface roughness forming blisters. This controllably shifts the wetting behaviour towards a hydrophilic or hydrophobic regime[8] depending on dose.

We will present a overview of the research, expanded by new data from ice-adhesion and drop impact investigations. The results may be beneficial for steam turbine blades, enhancing water droplet removal, and wind turbine blades, potentially delaying the ice formation. Gradients also could be applied in microfluidics, for example, lab-on-a-chip applications.

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I5A.1 Linear to Circular Bioeconomy – New Zealand's opportunities and challenges in the 21st century

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5A | Replacement materials, Bay Trust Forum, February 9, 2023, 2:00 PM - 3:40 PM

How do you create a world without waste, where value stretches beyond monetary value? On the journey towards true sustainability – economy, environment and society must work together not against each other. Scion's 2030 Strategy is simply summed up in 9 words - Enabling New Zealand to transition to a Circular Bioeconomy! This presentation will outline how Scion technologies and innovations can lead not only to a post Covid19 economic re-build but a fundamental shift. Specific focus will be on plastics and value adding to primary industry side and waste streams – both examples for the challenges and opportunities that arise through the transition to a circular bioeconomy. Considering the ongoing sustainability discussions around plastics, it is easy to forget that the use of plastics in several sectors has resulted in improved health, energy savings, increased crop production, improved food quality, reduction of food waste as well as the improvement of the overall ecological footprint. This is critical for a world that is facing challenges like feeding 10 billion people by 2050, a plastic waste flood & reduced availability of finite resources.

I5A.2 The Scientific Basis of Our Reactive Metals Based Civilization

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5A | Replacement materials, Bay Trust Forum, February 9, 2023, 2:00 PM - 3:40 PM

Our civilization is based upon the reactive metals. All these metals and their alloys react with oxygen and water with considerable negative changes in the Gibbs energy, indicating that the reactions are thermodynamically spontaneous and many of the reactions occur at considerable rates; some violently so (e.g., the burning of Al or Mg in air). Corrosion in aqueous systems is an electrochemical process comprising at least two partial reactions, one for the electrodissolution (destruction) of the metal substrate to produce electrons that are quantitatively consumed by a cathodic partial reaction, such as the reduction of oxygen or the evolution of hydrogen. Fortunately, once the potential exceeds a critical value, known as the Flade or passivation potential, the rate drops precipitously to values that are sufficiently low (< 1 μm/a) that the metals and their alloys may be used to fabricate machines that retain their precise dimensions over useful service lifetimes (40 – 100 a). This is known as the passive state in which the thermodynamically highly reactive metals attain kinetic stability because of the formation of a 1-3 nm thick metastable oxide film on the surface. In this presentation, I will review the scientific basis for the phenomenon of passivity within the framework of the Point Defect Model (PDM) and define precisely the condition that must be achieved for passivity to occur. Indeed, the occurrence of our metals-based civilization can be expressed as a simple inequality that has profound implications for life as we know it

5A.1 Harvesting (and Using) Motion via Polymers

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5A | Replacement materials, Bay Trust Forum, February 9, 2023, 2:00 PM - 3:40 PM

By 2050, it is estimated that there will be over 100 billion devices connected to the internet. Over 50% of these are anticipated to be wearable, implantable, or remote devices. In order to power these devices, larger (higher energy density) batteries will be needed – however, this will lead to large footprint, heavy devices. Harvesting ambient (from motion, heat, and/or light) energy via ferroelectric materials will emerge as a critical tool to supplement battery power, thus mitigating increases in battery size.

We have recently reported record efficiency ferroelectric polymer energy harvesters enabled by polarisation locking of polyvinylidene difluoride-co-trifluoroethylene (PVDF-TrFE) around a nanomaterial template [1]. We use this PVDF-TrFE energy harvester, as well as novel 2D ferroelectric materials [2], as models to study ambient energy harvesting. This talk will delve into the complexity of energy harvesting from ambient energy, discussing the interplay between thermal, photon, and mechanical energy harvesting in ferroelectric polymers [3,4]. We then demonstrate the ability to couple these ambient energy harvesters directly with functional catalysts [5], enabling low overpotential electrocatalysis for both pollutant degradation and water splitting, in addition to charging electrochemical energy storage devices.

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5A.2 A circular approach to valorize greenhouse tomato by-products in biobased and biodegradable injected materials for horticulture sectors

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5A | Replacement materials, Bay Trust Forum, February 9, 2023, 2:00 PM - 3:40 PM

Due to their good mechanical properties despite their relatively low weight, plant fibre composites are being used in an ever-increasing number of industrial applications (1). This study focuses on the use of tomato (Solanum lycopersicum L.) industrial by-product biomass as reinforcements for designing a range of new injectable materials with either conventional petrobased, biobased or biodegradable polymers matrix. After a deep morphological study of the tomato reinforcing particles through SEM and dynamic analysis, mechanical characterization was carried out on the designed formulations. Our mechanical results demonstrate that this circular approach is of interest for composite applications since the performances obtained are compatible with current applications. The tomato by product-reinforced materials can compete with existing formulations and according to the matrix and particles morphology, it is possible to offer a large range of products, fully biobased or biodegradable or not, depending of the targeted application.

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5A.3 Ball-Milling for the Green Synthesis of Metal-Organic Frameworks: a Design-of-Experiment Approach

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5A | Replacement materials, Bay Trust Forum, February 9, 2023, 2:00 PM - 3:40 PM

The development of solvent-minimised synthesis is crucial to decreasing dependence on traditional hazardous routes of metal-organic frameworks (MOFs)[1]. This work explored the green synthesis of a copper trimethyl 1,3,5-benzenetricarboxylate (CuBTC or HKUST-1) MOF using mechanochemical synthesis by ball milling. Here, we employed a design-of-experiment (DoE) approach to explore the reaction mechanism and optimise the MOF formation. In this study, the mechanochemical-driven MOF samples were fully characterised by X-ray powder diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), Transmission electron microscopy (TEM), scanning electron microscope (SEM) and gas adsorption. The XRD and FT-IR results demonstrate the successful synthesis of CuBTC. SEM images indicate that the particle size of the synthesised MOF samples is between 0.6 µm and 0.9 µm. Interestingly, the mechanochemical synthesis reached a higher yield of 24% than 4% yield from the solvothermal counterpart although the crystal size was slightly smaller. This study is a good showcase for the advantages of mechanochemical synthesis in the rapid preparation of CuBTC, suggesting the development of the green and upscalable synthesis with potential industrialisation promising.

5A.4 Bioactive biomaterials derived from chitosan for active and sustainable food packaging

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5A | Replacement materials, Bay Trust Forum, February 9, 2023, 2:00 PM - 3:40 PM

Background: Bioactive chitosan is a functional biomaterial derived from marine sources, namely chitin through a deacetylation process1. Chitosan possesses excellent functional and biological properties such as biocompatibility, biodegradability, antioxidant and antimicrobial ability, film forming capacity, and environmental friendliness2. Due to its outstanding functional characteristics, chitosan, and its derivatives chitooligosaccharide (COS) demonstrate good bioactive properties, which have been gaining attention globally as potential biomaterials for the development of active and sustainable food packaging3.
Aim: In the present study, bioactive COS is coupled with chitosan and other biomaterials to prepare an active film for the preservation of perishable foods, including fish, meat, fruits, vegetables, and dairy products.

Method: Bioactive COS was prepared using microwave-assisted processing technique developed by our team4. Chitosan, COS, and bioactive biomaterial solutions were developed separately for the formulation of casting solutions. The inter-mixed blend was stirred at room temperature for 1 h to prepare a homogeneous solution and cast in petri dishes to obtain active films. The physical, mechanical, antioxidant, antimicrobial, barrier, optical, and structural properties (scanning electron microscopy and Fourier transform infrared) of active films were investigated.

Results/conclusion: The physicochemical and microbial properties such as water vapor permeability, elongation at break, tensile strength, antioxidant activity, and antimicrobial capacity against Escherichia coli of the active film. The addition of COS and other biomaterials to the chitosan matrix significantly improved antimicrobial efficacy. The results suggest that the developed active film could be considered as a sustainable food packaging for the preservation of perishable foods.

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I5B.1 Zero-CO2 ironmaking in a hydrogen fluidised bed

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5B | Catalysis 4 - carbon mitigation, Skellerup, February 9, 2023, 2:00 PM - 3:40 PM

The global steel industry emits >3Bt CO2 per annum, comprising ~ 7% of total global GHG emissions. The primary culprit is the initial ironmaking process, in which oxide ores are chemically reduced to iron metal using fossil-based carbon. Eliminating this emissions-source requires an alternative reaction process – and hydrogen-reduction is emerging as the most viable future route. This could use 'green hydrogen' generated from renewable energy to achieve 'near-zero-CO2' ironmaking at industrial scale.

New Zealand's national electricity supply is > 85% renewable, making it an attractive location for both green hydrogen production, and a hydrogen direct reduced iron plant (H2-DRI). This talk will discuss results from our ongoing research programme investigating a new fluidised bed process for the hydrogen reduction of NZ's indigenous titanomagnetite ironsand ore.

At present, fluidised beds are not widely favoured for the reduction of iron ore fines, as they are known to be susceptible to 'sticking' during reduction with methane or syngas. This 'sticking' causes sintering of the bed and arrests the reaction. However, we have shown that titanomagnetite ironsands can be fully reduced without the onset of sticking in a laboratory fluidised bed, even at temperatures above 1000C. This surprising behaviour is due to the formation of a thin encapsulating Ti-rich oxide shell around each particle, which prevents metal-metal contact at the particle surfaces. The formation mechanism of this micro-morphology will be discussed, along with its implications for the potential development pathway for H2-DRI industry in NZ.

I5B.2 Electrochemical Reduction of Carbon Dioxide

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5B | Catalysis 4 - carbon mitigation, Skellerup, February 9, 2023, 2:00 PM - 3:40 PM

Sustainable technologies focused on carbon dioxide utilisation are essential if we are to shift to new sources of energy supply and mitigate climate change. Among the technologies developed so far, those based on electrochemistry, which utilize electricity from intermittent renewable sources as the energy input, are particularly attractive since they offer excellent scalability for industrial implementation. Commercially feasible electrochemical processes for carbon dioxide utilisation require the use of highly stable, selective and active catalysts to overcome high energy barriers associated with the relevant reactions. In recent years, nanoengineering strategies have been applied to develop more advanced electrocatalysts.1,2 With the assistance of advanced instrumental characterization tools and more sophisticated density functional theory calculations, significant progress has been made in the development of advanced electrocatalysts.3,4 To fully realize the potential of electrochemical CO2 reduction technology for commercial application, more advanced gas diffusion electrodes have been developed.5 This talk highlights the recent progress in the electrode/electrocatalyst design and mechanistic study made by the Monash Electrochemistry Group.

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5B.1 Carbon Dioxide Conversion Using Low Melting point Gallium Magnesium Liquid Metal Alloys

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5B | Catalysis 4 - carbon mitigation, Skellerup, February 9, 2023, 2:00 PM - 3:40 PM

The need for effective and adaptive technologies for carbon dioxide (CO2) mitigation targeting global net-zero carbon emissions is critically growing. Hence, innovative technologies for CO2 reduction have attracted worldwide interest from scientific research communities. The use of liquid metals for the conversion of CO2 into carbon or solid carbonaceous products has gained increasing attention in recent years due to their high activity and resistance to coking. Here, we present a facile approach for the reduction of CO2 to solid carbon at/and near room temperature, and atmospheric pressure, using Mg-Ga liquid metal alloys. In this process, Mg plays a major role in driving the dissociation of CO2 to its elemental constituents, carbon and oxygen. During the reaction process, Mg ions diffuse to the gas-liquid interface and reduce CO2 to carbon while undergoing an oxidation reaction. The electrochemical method ensures a sustainable cyclic process by reducing Mg ions back to their metallic counterpart. The use of liquid metal alloys for CO2 reduction reactions could enable us to achieve CO2 capture and storage at room temperature, setting a new foundation for the future exploration of efficient CO2 mitigation issues.

5B.2 Electrochemical CO2 extraction from seawater

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5B | Catalysis 4 - carbon mitigation, Skellerup, February 9, 2023, 2:00 PM - 3:40 PM

Climate change, driven by rising concentrations of greenhouse gases in the atmosphere, is already starting to cause widespread damage and increasing concern to the general population (1). Carbon dioxide (CO2) is the single largest anthropic contributor to global warming. Hence, research and development focused on removing CO2 from the atmosphere is a key aspect to the goal of achieving a carbon zero balance. Among various methods, electrochemical capture and conversion of CO2 are gaining attention thanks to their flexibility and efficiency. Nevertheless, a majority of the early stage of studies are performed based on small scale due to the high cost of synthesized electrodes for CO2 capture or conversion. In addition, the high energy cost of direct air capture remains challenging for wide application (2). Instead of extracting CO2 directly from air, the higher abundance of CO2 in seawater provides an attractive source for CO2 extraction (3).

Inspired by water softening techniques (4-5), CO2 can be extracted from seawater based on seawater electrolysis and mineralization. The advantages of this method include: single-step direct mineralization of CO2, relatively good energy efficiency and reduction of ocean acidification. Moreover, this method is promising for very large scale CO2 extraction. In this work, results from electrochemical CO2 extraction and mineral precipitation from real seawater will be described.

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5B.3 Data-Driven Structure-Function Mapping of Organic Solar Cell Materials

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5B | Catalysis 4 - carbon mitigation, Skellerup, February 9, 2023, 2:00 PM - 3:40 PM

Low-cost solar cell materials are crucial for curbing our reliance on fossil fuels and for space exploration. Solar cells based on organic materials have had some success, however further improvements in their solar efficiencies have been hindered by their complex nanoscale structures [1]. This complexity is preventing us from fully understanding the physical mechanisms governing overall solar efficiencies.

Organic solar cells have recently shifted towards crystalline molecular materials [2]. This simplifies the nanoscale structures of organic solar cell materials, allowing us to model the kinetics of energy and charge migration processes using simplified computational techniques.

In this talk, we present a database developed in-house, containing intermolecular excitonic couplings of thousands of OPV crystal structures from the Cambridge crystal database [3]. These couplings can be used to predict key parameters for solar cells devices, such as energy and charge diffusion lengths. Using these parameters, we aim to build a structure-function relationship for organic solar cell materials and provide a path towards computational material design for solar cells, similar to that used in modern drug discovery.

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5B.4 Quantum dots and extracellular vesicles as detection strategies for disease and bacteria

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5B | Catalysis 4 - carbon mitigation, Skellerup, February 9, 2023, 2:00 PM - 3:40 PM

Recent work has suggested that increased mobility of a catalyst enables a dynamic interaction between the catalyst and reactant species which enhances catalytic performance[1-4]. With the understanding that catalysts can be dynamic species, a logical next step is to develop catalysts with in-built dynamic functionality.

Liquid metals are dynamic[5] and self-healing[6] materials. The application of liquid metals to catalysis could allow a more fluid-like interaction between the catalyst and the reactants and also the ability to reform the original catalyst after desorption of the reactants. Ga is the ideal candidate for a liquid metal catalyst as it has a low melting point (302.9 K) and is non-toxic making it appropriate for real-world application. Furthermore, Ga has the widest liquid temperature range of any element[7], meaning that the liquid properties of Ga are accessible under a variety of different reaction conditions. While Ga in isolation is inactive[8], it readily alloys with many other elements, therefore the properties of the liquid metal system can be tuned.

In this work, the idea that nanoscale Au exhibits good catalytic activity[9] is combined with the emerging requirement of having a dynamic interaction between catalyst and reactants. Through extensive ab initio molecular dynamics simulations, the structures of liquid GaAu systems under likely experimental conditions at a range of Au concentrations are examined. A hypothesis for the observed behaviour of these different Au concentrations is also proposed.

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I5C.1 Quantum dots and extracellular vesicles as detection strategies for disease and bacteria

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All living cells release spherical membrane-enclosed entities called extracellular vesicles that mimic the cell they came from. Extracellular vesicles have the potential to serve as alternative targets to whole cells allowing for bacteria detection or can as detection markers for disease. The small nano-size of extracellular vesicles as compared to the cell they originated from allows for easier conjugation to targeting ligands used for detection strategies. More importantly, evidence of many extracellular vesicles in extracellular milieu is of particular significance as they can offer an abundance of target sites for detection. With the given benefits, our group aims to use extracellular vesicles and customise nanoparticles as promising markers for detection of pathogens and diseases using strategies developed within our group. For example, we aim to detect Escherichia coli bacteria by detecting their extracellular vesicles using a sandwich ELISA based platform. Highly specific DNA aptamers are used to target Escherichia coli-derived extracellular vesicles. These aptamers are conjugated to InP/ZnS quantum dots to enable a fluorescence-based detection. A similar strategy uses a gold substrate and electrochemical impedance spectroscopy to capture breath-derived extracellular vesicles for lung cancer detection. Once disease specific extracellular vesicles are capture, an electrical response confirms the detection, potentially creating a disease breathalyser. Using nature's own nanoparticles combined with nanotechnology, our group aims to develop novel strategies for detection of pathogens and disease.

I5C.2 Novel conducting polymers biointerfaces for bioelectronics

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Conducting polymers (CPs) have been widely used as electroactive biointerfaces in applications such as electrically stimulated tissue engineering and flexible organic bioelectronics. In this talk, several different approaches to advanced electroactive biointerfaces based on CPs will be presented.

The first approach addresses the issue of poor solubility and processability of CP by functionalization of CPs with various moieties by grafting of CP backbones with polymeric sidechains. That enables modification of optoelectronic, physical and mechanical properties of the CPs and their use as biomimetic conductive biointerfaces.[1]

The second approach addresses the issue that electrodes used in tissue recording and stimulation are commonly 2D and made of rigid conducting materials that cannot adequately probe the actual 3D cell environment within tissues. Our approach to overcome that is based on a precise fabrication of individually addressable, high aspect ratio, soft and flexible 3D CP-pillar microelectrode arrays by means of 'direct 3D writing'. Such 3D microelectrode arrays could be employed in a variety of applications, from biological sensing to recording and electrically stimulating cells and tissues [2], with the array design easily adjustable. The third approach to electrochemically addressable biointerfaces is based on flexible, microporous, electrochemically switchable membranes that can selectively and efficiently capture, and then non-destructively release, cancer biomarkers, such as cancer cells-shaded extracellular vesicles (EVs) [3] and rare cancer cells [4] Such EVs and cells captured from large volumes of complex biological samples and released into clean and small volumes of buffers could be used for further analysis, for example, for medical diagnostics.

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5C.1 Biodegradable piezoelectric nanogenerators from biological materials

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Clean and renewable energy resources are in demand to meet the global challenges of energy shortage and environmental pollution.1 Piezoelectric nanogenerators have attracted great attention for generation of clean and renewable energy through harvesting mechanical energy from sustainable environmental resources e.g. wind, wave, rain, tides and human/animal motion.2 However, the most widely used piezoelectric materials are made of inorganic components or synthetic polymers, which provide one or more challenges related to being rigid, brittle, non-degradable or toxic, thus limiting their practical applications. Piezoelectric biomaterials, e.g. amino acids, peptides, proteins, cellulose, viral particles and tissues are naturally biocompatible, degradable, available from environmentally sustainable resources and in many cases have the capability to be processed as flexible materials. Although these biomaterials have been reported to be inherently piezoelectric, owing to their permanent dipoles, their bulk bio-piezoelectric output is extremely low, which is mainly due to the lack of, or poor large-scale assembly and domain aligning as well as large heterogeneity within biological structures.3, 4 Moreover, the correct piezoelectric response measurement of biological materials is extremely complicated with their low piezoelectricity and the interference from other change generation sources such as contact electrification.5 This project aims to develop strategies to measure the low piezoelectricity of biological materials and using that knowledge to identify the lead candidates among a wide variety of biological materials. In addition, the project exploits the feasibility of different chemical and structural modification techniques to enhance the assembly and domain alignment in biological materials, thus improving their bulk bio-piezoelectric output.

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5C.2 Synthesis and characterization of antimicrobial colloidal polyanilines

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Polyaniline (PANI) is a well-known antimicrobial polymer that has been studied widely. However, it has certain limitations, including its processability (for scale-up) and limited antimicrobial potency. Therefore we co-polymerised aniline with 3-amino benzoic acid to overcome this limitation [1]. However, it has been reported that PANI showed better activity than 3ABAPANI [1]. Consequently, we modified the PANI and 3ABAPANI colloid for improved activity by incorporating Ag nanoparticles (AgNP) into the polymer by direct reduction of Ag+ (1.5mL, 10mM) by PANI and 3ABAPANI [2]. The amount of AgNP present in PANI-Ag and 3ABAPANI-Ag colloids is estimated using Inductively coupled plasma mass spectrometry (ICP-MS) analysis. The shift in physical properties after incorporating AgNP is measured using particle size and zeta potential analysis (determine particle size and stability of colloids), UV-Vis absorbance, and FTIR spectroscopy. The MBC values of the colloids against Escherichia coli are recorded after different time intervals (10 min, 30 min, 6 h, and 24 h). Thereafter, the observed antimicrobial activity of PANI, 3ABAPANI, PANI-AgNP and 3ABAPANI-AgNP is tested and compared with the same amount of AgNP synthesised using Ag+ (1.5mL, 10mM) reduction using sodium borohydride. We observed that addition of AgNP halved the MBC values against E. coli for both PANI and 3ABAPANI.

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5C.3 The exploitation of dynamic S-S bonds in 50-poly(S-r-DCPD) for erasable data storage and encoding messages

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Fully crosslinked Sulfur-based polymers offer a range of advantageous properties due to the dynamic nature of S-S bonds. Previous work by Mann[1] has identified a simplistic method to form a copolymer made from a 50:50 weight ratio of waste Sulfur and DCPD, which has shown to have extensive applications, such as acid and solvent resistant coatings[1], as a mercury sorbent[1] along with properties such as high hardness and modulus. This research presents a proof of concept using this polymer and resulting composites with y-Fe_2O_3 nanoparticles to provide a material ideal for scanned probe nanoindentation data storage and lithographic applications. This study demonstrates the polymer as a non-volatile memory medium, using conventional atomic force microscopy to create nanoscale indents by physical material displacement, where the depth of indentation is utilized as another dimension forming a more diverse range of encoding methods. Erasure of the data is shown by heating the polymer to between 140^{o}C and 170^{o}C, where the dynamic nature of the S-S bonds is exploited to regenerate a re-writable surface. The resulting shelf stability of the data has been monitored over a period of six months in ambient conditions to show no loss of indentation depth over time. This polymer and technique could be used as a more ecologically friendly, cheaper, and lower energy expenditure alternative to the traditional thermomechanical nanoindentation[2-4] and existing media for non-volatile memories[5] leading to the development of the next generation of data storage media and more private modes for encoding messages.

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5C.4 Conductive composites of an elastomeric biopolyester and their application in 3D printed sensor devices

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Substituting petroleum-based plastics with renewable bio-based materials is one key element in establishing a circular economy and is necessary in combating global climate change. Poly(3-hydroxyalkanoates), polyesters obtained from bacterial fermentation, represent one of the most promising classes of bioplastics with potential future uses in food packaging, tissue engineering and biomedical applications [1-3]. In this work, poly(3-hydroxyoctanoate), a biocompatible polymer with a skin-like feel [4], is compounded with carbon nanofibers (CNF) or carbon black (CB), respectively, to form flexible, 3D printable, bio-based conductive composites. Conductivities up to 10 and 3 S/m can be achieved for CNF and CB, respectively, without negatively affecting the composites' processability. Both filler materials act as nucleating agents for PHO crystallization, significantly accelerating this process which is extremely slow for the filler-free polymer. Mechanical performance, e. g. elastic modulus, is also improved by the addition of CNF or CB. Both types of filler form composites that show a distinct response to mechanical deformation: bending, twisting and stretching (up to 10 % elongation) result in a marked decrease of their electrical resistance (up to 30 %). This phenomenon has been exploited to fabricate a 3D printed strain sensor that can detect flection and extension via a change in resistance. Our results demonstrate the potential of this sustainable biopolymer and its composites for applications in the biomedical space.

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I5D.1 Interfacial Energetic Landscape in Non-fullerene Acceptor Organic Solar Cells and its Impact on Device Performance

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In bulk heterojunction organic solar cells, the energetic landscape at the donor-acceptor interface provides the driving force for charge separation. The mechanism leading to efficient charge separation in fullerene-based blends has been intensively investigated, however with the recent advent of high-efficiency non-fullerene acceptors (NFAs) now surpassing 19% power conversion efficiency, the previous findings have to be revisited for NFA-based systems. In this presentation, I will discuss our latest insights into the photophysical processes governing charge separation, recombination, and energetic (voltage) losses in novel NFA-based systems studied by steady-state and advanced transient spectroscopy techniques. I will address the question, how the interfacial energy offsets control exciton dissociation and charge separation in binary and ternary blends of polymer or small molecular donors with novel NFAs, including photoactive layers using state-of-the-art Y-type acceptors. Generally, it appears that it is primarily the ionization energy (IE) offset that limits the exciton-to-charge transfer (CT) state conversion in many low-bandgap NFA-based systems, while the subsequent separation of the CT state into free charges is barrier-less. Sizeable IE offsets of 0.4-0.5 eV are required to ensure quantitative exciton-to-CT state conversion. The underlying reasons of this limitation, their implications for future donor and acceptor material design strategies, and novel computational (in-silico) approaches to material design will be discussed.
Refs.: Nat. Mater. 2021, 20 (3), 378-384; Adv. Energy Mater. 2021, 11 (28), 2100839; Adv. Energy Mater. 2021, 2102363;

I5D.2 Accumulation of Dark Excitons in Thin Quasi-2D Perovskites Limits Amplified Spontaneous Emission

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Quasi-two-dimensional (Q2D) perovskites, composed of mixed layered quantum well structures, are emerging as competitive materials for highly efficient light-emitting diodes and lasing applications. Their stability and excellent optoelectronic properties, including the potential for carrier concentration via energy transfer, make them excellent candidates for these applications. However, their excitonic nature also brings the possibility of parasitic losses from quenching by triplet excitons, one of the major losses limiting continuous wave and current injection lasing from organic semiconductors. While it has been claimed that the presence of dark triplet excitons in perovskite semiconductors is responsible for the observed lasing death phenomenon, no detailed mechanism has been laid out and additionally recent key studies[1,2] reported contradictory results on the role of triplet excitons in lasing degradation for similar layered perovskites films.

Here, a tunable repetition fibre laser amplifier was used to control the concentration of accumulated triplet excitons in combination with ultrafast broadband transient photoluminescence spectroscopy[3] to directly monitor the singlet-triplet annihilation of the bright singlet state population on a sub-picosecond timescale. This unique method is used to determine the role of out-of-plane confinement on the triplet exciton stabilisation in Q2D domains and the mechanism involved in averting population inversion in mixed Q2D perovskite films through the accumulation of long-lived triplet states in highly excitonic Q2D perovskite domains. These findings not only advance the fundamental understanding of energy transfer pathways in perovskite nanostructures, but also establish urgently needed design rules for highly efficient and stable lasers and light-emitting diodes.

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5D.1 Performance Evaluation of Solid State Luminescent Solar Concentrators based on InP/ZnS–Rhodamine 101 Hybrid Inorganic-Organic Luminophores

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Luminescent Solar Concentrators (LSCs) suffer greatly from reabsorption, where emitted light is parasitically reabsorbed by a luminophore. Specifically designed luminophores with inherently large Stokes shifts have been successfully synthesised in the literature, however they introduce a new issue of poor absorption due to excessive blue shifting of the luminophores' absorption. Hybrid luminophores consisting of quantum dots (QDs) coupled to organic dyes offer a solution to this problem, by improving light sensitisation and increasing the Stokes shift via energy transfer. We present a Cd/Pb-free InP/ZnS QD donor coupled to a Rhodamine 101 acceptor hybrid luminophore LSC, giving a mean 33% increase in external quantum efficiency relative to InP/ZnS QDs by themselves. This study represents the first inorganic/organic hybrid nanomaterial system with attached luminophores in the solid state. We also perform an in-depth investigation by optical characterisation of the different operational metrics of our novel LSCs.

5D.2 Theoretical studies of thermally activated delayed fluorescence (TADF) emitters: Exciplex-type and multiple resonance type emitters.

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The thermally activated delayed fluorescence (TADF) phenomenon includes an effective conversion from the triplet excitons to the singlet ones, followed by the delayed fluorescence. This allows the full use of triplet excitons in organic light emitting diodes with purely organic molecules. In this regard, tremendous attention has been given to the phenomenon.[1-2] The spin-orbit couplings for this singlet-triplet conversion in TADF emitters remain marginal. Therefore, the energy difference between the singlet and triplet excited states, ΔEST, is desired to be minimal.

In recent reports, exciplex-type emitters show highly efficient TADF to which through space (TS) charge transfer (CT) is often attributed. However, it remains elusive as to why TSCT emitters are more efficient in TADF than conventional emitters of through-bond CT. Without resorting to these vague notions, we will present the role of exciton binding energy, which provides a simpler and more straightforward insight into the relationship between the molecular topology and ΔEST. [3]

In addition, multiple resonance type TADF emitters containing B atom, namely, DABNA derivatives, recently attracted massive attention. Although it has sizable ΔEST of ca. 0.15 eV, these molecules exhibit considerable TADF emissions. In this talk, we will present our recent results on the mechanism of effective reverse intersystem crossing in this molecule where non-Condon type vibronic coupling between the T_1 and T_3 state plays a major role.[4]

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5D.3 High-performance colorful semitransparent organic solar cells

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Semitransparent organic solar cells (STOSCs) are a technology that combines the benefits of visible light transparency and light-to-electrical energy conversion. One of the greatest opportunities for STOSCs is their integration into windows and skylights in energy-sustainable buildings. For this application, the aesthetic aspects of solar cells may be as important as their electrical performance. Here, our strategy enables to achieve high-quality and colorful STOSCs using Fabry-Pérot etalon-type electrodes. These electrodes are composed of an antimony oxide (Sb2O3) cavity layer and two thin Ag mirrors. These dichroic tri-layer structures perform two functions as top conducting electrodes and color filters. These dual-function electrodes were applied to photovoltaic devices and displayed vivid colors, natural transparency, and good performance as compared to devices that use conventional metal electrodes. Furthermore, to achieve saturated colors and low photocurrent losses, active layer materials were selected such that their transmittance peaks matched the transmittance maxima of the electrodes. These strategies for colorful STOSCs result in power conversion efficiencies (PCEs) of up to 13.3% and maximum transmittances (TMAX) of 24.6% in blue devices, PCEs of up to 9.71% and TMAX of 35.4% in green devices, and PCEs of up to 7.63% and TMAX of 34.7% in red devices.

5D.4 Ruddlesden-Popper Mixed-Dimensional Perovskites for Triplet-Triplet Annihilation and Singlet Fission

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The maximum theoretical power conversion efficiency (PCE) of photovoltaic (PV) cells is severely limited due to the exclusion of sub-band gap photons and the rapid thermalisation of hot-carriers, as described by Shockley and Queisser in 1968. (1) The region of excluded sub-band gap photons can be reduced by utilising triplet-triplet annihilation (TTA) to combine the energy of multiple photons into emissive singlet excited states. Thermalisation can be reduced via singlet fission (SF), which can redistribute the energy of photons with twice the band gap energy over two triplet excited states.

To make use of either of these processes requires coupling TTA or SF capable chromophores to another chemical species to either supply triplets for TTA or to accept triplets produced via SF. Inorganic semiconductors have been shown to be suitable for this purpose, however, the overall efficiency of these hybrid materials remains low due in part to weak interactions between the organic and inorganic components, resulting in inefficient/non-existent triplet energy transfer (TET). (2) My work focuses on trying to address this issue by incorporating TTA/SF capable molecules into the structure of Ruddlesden-Popper mixed dimensional perovskites, resulting in a single hybrid material. By tuning both the band gap of the perovskite and the choice of organic chromophore, these perovskites could potentially be utilised for both upconversion and singlet fission.

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I5E.1 External Stimulation Platforms for Stem Cell Fate Control

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5E | Bio 5 – Engineered environments and characterisation, Sigma, February 9, 2023, 2:00 PM - 3:40 PM

Tissue engineering is a field which has applications for many healthcare solutions requiring the generation of new tissues, including cardiovascular repair, wound repair, and bone regeneration. Patient derived stem cells present the opportunity to deliver targeted, tailored, and autologous tissue; by developing new approaches to direct the fate of adult stem cells, we can improve the efficacy of using these stem cells in tissue engineering.

External physical stimulation has demonstrable influence on stem cell fate, and can be delivered both via a stimuli-responsive biomaterial or by interfacing directly with the cell. [1]

External physical stimulation, such as electrical or acoustic, directs human mesenchymal stem cell (hMSC) differentiation, without exogenous growth factors, towards different cell tissue types. [2]Optimising the design and integration of the external stimulation approach with biomaterials is a key step forward in personalised tissue engineering.

Here I will present my research platform which explores the dynamic response of stem cells to external stimulation combined with supportive passive biomaterials. Different biomaterials, both new (thermoresponsive bioink) and clinically relevant (diamond coated titanium), are studied with 'pre-conditioned' (stimulated) stem cells to explore new methods to deliver effective and efficacious tissue engineering using adult stem cells.

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I5E.2 Directing the differentiation of stem cells using cell-imprinted culture platforms

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5E | Bio 5 – Engineered environments and characterisation, Sigma, February 9, 2023, 2:00 PM - 3:40 PM

Directing the differentiation of stem cells into specialized cell types in the lab has huge therapeutic potential. Producing specific cell types to study treatment for diseases, or using them for tissue repair and cell-based replacement therapies, are some of these benefits. Most of current methods for in-vitro stem cell differentiation, such as the use of specific extracellular matrices or defined culture media compositions, are expensive and not 100% effective in most cases. In recent years, engineering cell-culture substrates and the use of surface topography have become more popular as alternative ways to induce stem cell differentiation [1, 2]. Some studies have used cell-imprinted pit-like surface features as surface topography [3-5].

In this work, polystyrene (PS) culture platforms with pit-like and raised cell-imprints (negative and positive bioimprints) were used to study the role of surface topography on differentiation of stem cells. Bioimprints are a 3D replica of cellular morphology onto a rigid material and they have all the cellular details down to nanometer scale. An advantage of using positive bioimprints as surface topography, is that they can mimic the physical shape of cells' natural environment, without any biological cues.

Semi-differentiated mouse myoblast cell line (C2C12 cells) were seeded and grown on the PS films (patterned and flat). C2C12 myoblast have a fibroblastic morphology, but when myoblasts become confluent and under low serum conditions, they diffuse into one another and differentiate into elongated multinuclei myotubes with a very different morphology. The goal of this study is to demonstrate the differentiation level of C2C12 cells on imprints of myoblasts vs myotubes.

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5E.1 Gelatin methacryloyl microspheres to enhance the survival and maturation of directly reprogrammed neurons for cell replacement therapy in Huntington's Disease

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Cell replacement therapy is considered a potential treatment for Huntington's Disease (HD). The advances of human-derived neural stem cells have attracted much attention within the field as a potential source of cells for transplantation (Rosser & Bachoud-Levi, 2012). Direct cell reprogramming to generate induced brain stem cells from human skin cells offers an exciting alternative to the use of human fetal tissue or pluripotent stem cells for cell replacement therapy (Connor et al., 2018).

While cell replacement therapy holds great potential as a treatment for HD, the current delivery of cells in liquid suspension leads to poor cell viability and functionality, impeding clinical translation (Foster, Marquardt, & Heilshorn, 2017). There is increasing interest in gelatin methacryloyl (GelMA) hydrogels as a three-dimensional (3D) scaffold for cell transplantation as it mimics the 3D in vivo microenvironment with low immunogenicity (Liu, Weng, Zhang, Sun, & Yang, 2020). This technology allows for the generation of micro-sized spherical hydrogels (microspheres) (Saralidze, Koole, & Knetsch). We propose that encapsulation of directly reprogrammed induced brain stem cells in GelMA microspheres will enhance cell replacement therapy by augmenting transplanted cell survival and promoting brain cell differentiation and integration.

GelMA microspheres were fabricated using a flow-focusing microfluidic device and were used to encapsulate directly reprogrammed human brain stem cells. To enhance the survival and differentiation of the cells following transplantation, we investigated loading brain-derived neurotrophic factor (BDNF) into the GelMA microspheres. Future work will investigate the capacity of human brain stem cells encapsulated in GelMA microspheres to generate replacement brain cells and improve functional impairment following transplantation into a rat model of HD. This work will provide a unique strategy for cell replacement therapy to treat HD.

5E.2 Biomolecule incorporation and release from engineered biointerfaces for cell behavioral studies.

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Cells have shown to interact and respond with their surroundings through physical and biochemical cues. Biointerfaces for presentation of biomolecules to cells have garnered much attention in recent literature[1], with cells responding best to a controlled release - mimetic of biomolecule presentation by the extracellular matrix[2]. The signalling pathways, however, are still not entirely understood, and experimental systems that allow de-coupling of signalling pathways are lacking. Therefore, we investigate two systems for their ability to store and release biomolecules for eventual cellular studies. The first of these systems is block copolymer thin-films. In this study, we self-assembled PS-b-PEO in the presence of fluorescently labelled protein or peptide. The block copolymer self-assembles into a thin-film with a cylindrical hexagonal morphology, where the biomolecules become incorporated into the PEO cylinders. The release rate and amount were quantified using spectrofluorometry[3]. Due to difficulties controlling the release from the PS-b-PEO films, conducting polymer hydrogels were also explored as delivery platforms. This system combines the electrically actuating properties of polypyrrole with the low elastic modulus of poly(N-isopropylacrylamide), mimicking the naturally occurring extracellular matrix. pNIPAM-PPy was constructed with dodecylbenzenesulfonate (DBS) as the dopant and charged cargo as a co-dopant. Release of this cargo was analyzed quantitatively for both passive and active release. Cargo was shown to release passively significantly, with further quantities releasing actively on cue by reducing the conducting polymer hydrogel. Going forward, growth factors will be used as the cargo, and cell behaviour will be explored in response to the actuatable on-demand release.

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5E.3 Eutectic gels with 2D black phosphorus nanoflakes for antimicrobial treatments

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The rise of antimicrobial resistance among pathogenic bacterial and fungal cells has been declared one of the top 10 global public health threats by the World Health Organisation.[1] Recently, low-dimensional materials, including black phosphorous (BP), have emerged as promising antimicrobial agents. Previous studies have demonstrated that few-layer and 2D black phosphorus (BP) nanoflakes when applied as a surface coating, have a high effectiveness against a wide range of pathogenic microbial cells, whilst showing low toxicity towards mammalian cells.[2] One limitation facing BP as a surface coating is the rapid degradation under ambient conditions. To address this concern, BP nanoflakes were suspended into a green, non-toxic eutectic gel. The gel was able to delay the degradation of the BP nanoflakes, with the BP-gel still showing high antimicrobial activity. After one month of storage, BP-gel was able to achieve over 80% cell death against the model microbial cells methicillin-resistant Staphylococcus aureus (>80%), Pseudomonas aeruginosa (>97%) and Candida albicans (>95%). The combination of eutectic gel and few-layer BP nanoflakes provides a promising, practical pathway for implementing low-dimensional materials as next-generation antimicrobial treatments.

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5E.4 Characterisation of collagen: the use of synchrotron small-angle X-ray scattering (SAXS) and surface-enhanced Raman spectroscopy (SERS)

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Collagen is an abundant structural protein in mammalian animals including humans. Its native structure in biological tissues features a distinct hierarchical organisation which imparts a series of characteristic properties to the materials. To better understand various processes that construct, stabilise, and functionalise the collagenous native tissues and biomaterials, we used two advanced techniques, synchrotron small-angle X-ray scattering (SAXS) and surface-enhanced Raman spectroscopy (SERS), to reveal the structural insights during the processes.

Results from SAXS allowed us to understand the changes in the intermolecular arrangements associated with the chemical treatments (binding or crosslinking)[1, 2]. The SERS technique's excellent resolution in pinpointing changes in collagen functional groups is developed by our comprehensive studies to improve its reliability for accurate interpretations by minimising interferences in bioanalyses [2, 3].

Combining these techniques with the conventional protein analysis methods can reveal determinative factors in designing collagen-based materials, which supports researchers in this interdisciplinary field of physical and materials chemistry and biomedical sciences, as well as our partners in the advanced manufacturing industry.

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Pl.05 Active colloidal particles in nematics for physically intelligent micro-robotics and reconfigurable materials

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Plenary Session 5, Bay Trust Forum, February 9, 2023, 4:10 PM - 5:00 PM

Active colloidal particles in nematic liquid crystals are exciting vehicles for materials manipulation. Their shape and surface chemistry can be tailored to generate companion topological defects. Their motion can be tailored to drive far-from-equilibrium defect dynamics that generate new modes of motion and interaction based on nemato-elastic interactions and dynamics.

Given that colloidal scale objects are too small to carry computer chips, imbuing them with 'intelligence' is a major challenge in the field. We draw on soft matter concepts to develop physically-intelligent active colloidal systems that embed and dynamically reconfigure information in their nematic liquid crystalline milieu. This embedded information generates a diverse suite of physical interactions useful for manipulation of passive colloidal building blocks or colloidal cargo. Since these interactions rely on the colloidal cargo surface chemistry and not its material composition, the suite of interactions is materials agnostic, and can be used to build and reconfigure structures from diverse building blocks at multistable sites in the domain. This suite of interactions is particularly exciting in the inter-related realms of microrobotics and reconfigurable materials based on colloidal building blocks.

Our approach differs from existing approaches for reconfigurable devices that exploit nematic liquid crystal's optical birefringence. Should this approach gain traction, the opportunity for impact is tremendous, as society has made massive investment in the grooming of liquid crystalline responses, for example, in the over $160B/year liquid crystal display industry. While the display industry is now mature, the ability to build reconfigurable devices is ripe for new applications.

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K.17 Nanoporous materials with different functional elements: unique materials with multiple functions

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Keynote Session 17, Bay Trust Forum, February 10, 2023, 09:00 AM - 09:40 AM

Nanoporous materials with different functional elements are at the forefront in energy storage and conversion and environmental applications owing to their excellent photocatalytic and textural properties.1-6 In the first part of the talk, I will present about different ways of preparing a series of nanoporous materials with different chemical framework elements including carbons, carbon nitrides, boron nitrides and boron carbon nitrides, fullerenes and heteropoly acids with different structures, morphologies and pore diameters. I will also present how these materials will be effectively used for solving the global issues including carbon capture and conversion and the clean energy generation including hydrogen production using visible sunlight. Much focus will be given on the fabrication of mesoporous carbon nitrides with different molecular structures and nitrogen contents and their performances in energy storage and conversion, hydrogen production and oxygen reduction reaction. The change in the molecular structure of carbon nitride materials has significant impact on the final band gap and the basic properties which influence their performance in photocatalysis and energy storage.

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K. 18 Resolving the Light-Activated Processes of DNA Bound Transition Metal Polypyridyl Complexes Towards Imaging and Therapeutic Applications

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Keynote Session 20, Skellerup & WSP, February 10, 2023, 9:40 AM - 10:20 AM

DNA binding metal polypyridyl complexes show great potential as photodynamic therapy agents and for imaging and diagnostic applications. We have extensively studied the excited state dynamics of these processes for intercalating ruthenium dppz (dipyridophenazine) polypyridyl complexes bound to DNA.1-3 While the phenanthroline (phen) light-switch complexes can signal the presence of DNA, the tetraazaphenanthrene (TAP) complexes can cause photodamage by participate in direct one-electron photo-oxidation of guanine, which is sensitive to the local DNA environment and the binding orientation. In this talk I will discuss how time-resolved methods, including time-resolved infrared (TRIR) complemented by structural and computational studies, can be used to identify the binding site of photoactive metal complexes in solution, and to monitor sensitized DNA photo-oxidation. Finally, I will discuss our recent work that reveals that a ligand centered (LC) excited state and not the long-thought metal centered (2MC) state is responsible for the photo-oxidation of purine bases by intercalated chromium polypyridyl complexes.4

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K.19 Controlled assembly of retinal cells on fractal and Euclidean electrodes

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Keynote Session 19, Bay Trust Forum, February 10, 2023, 9:40 AM - 10:20 AM

Controlled assembly of retinal cells on artificial surfaces is important for fundamental cell research and medical applications. We investigate fractal electrodes with branches of vertically-aligned carbon nanotubes and silicon dioxide gaps between the branches that form repeating patterns spanning from micro- to milli-meters, along with single-scaled Euclidean electrodes. Fluorescence and electron microscopy show neurons adhere in large numbers to branches while glial cells cover the gaps. This ensures neurons will be close to the electrodes' stimulating electric fields in applications. Furthermore, glia won't hinder neuron-branch interactions but will be sufficiently close for neurons to benefit from the glia's life-supporting functions. This cell 'herding' is adjusted using the fractal electrode's dimension and number of repeating levels. We explain how this tuning facilitates substantial glial coverage in the gaps which fuels neural networks with small-world structural characteristics. The large branch-gap interface then allows these networks to connect to the neuron-rich branches.

I6A.1 Shedding light on skin cancers and skin diseases with Raman spectroscopy

Dr Michel Nieuwoudt[1,2,3,4], Dr Paul Jarrett[6], Dr Michelle Locke[7], Ms Hannah Matthews[1,2,3,4], Dr. Hannah Holtkamp[1,2,3], Dr Marco Bonesi[1,2,3,4,9], Mr Brydon Burnett[1,2], Dr Claude Aguergaray[2,3,9], Dr Satya Amirapu[10], Dr Angus Grey[11]

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6A | Nanomaterials and diagnostic devices, Bay Trust Forum, February 10, 2023, 10:50 AM - 12:50 PM

Raman spectroscopy is exquisitely sensitive to molecular vibrations which provide a fingerprint of their composition, structure in their environment within materials. This makes it an ideal technique for detecting differences and changes in the molecular composition of skin affected by skin cancers or skin diseases [1]. Additionally, it is non-destructive and can be applied in vivo using a portable system with fibre optic probe so ideal for use in a clinic.

By incorporating a Raman microscope this method can also be used for hyperspectral imaging of materials. It can also be combined with other analytical imaging techniques such as mass spectrometry with MALDI (Matrix Associated Laser Desorption Ionisation) to provide chemical image of the biomarkers in cross sections of diseased skin tissue.

This presentation describes our application of Raman spectroscopy in two different ways to investigate and diagnose different skin conditions and skin cancers.
Using a portable Raman device with custom fibre optic probe we measured 849 spectra of a wide variety of skin lesions and inflammatory dermatoses in vivo, in the clinic, from 320 individuals and used chemometric analysis of the spectra to classify the measured lesions as cancerous or benign.
We also investigated two skin diseases: Discoid Lupus Erythematosus (DLE), a common form of a cutaneous lupus disease, that causes permanent scarring, scarring, alopecia, hyper- or hypo-pigmentary change that particularly affects patients with skin of colour [2], and metallosis [3], by combining MALDI imaging with either in-vivo Raman measurements or Raman hyperspectral imaging.

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I6A.2 Exclusive liquid repellency enabled under-oil open microfluidic systems

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6A | Nanomaterials and diagnostic devices, Bay Trust Forum, February 10, 2023, 10:50 AM - 12:50 PM

We recently discovered a unique extreme wettability phenomena, named exclusive liquid repellency (or ELR). ELR allows, for the first time, inherent, absolute repellency of a liquid (i.e., with Young's contact angle = 180o) on a non-textured solid surface without the use of surfactants. We have begun to apply ELR across a range of applications. Central to our efforts is the creation of a new under-oil open microfluidic systems (UOMS) platform made possible by ELR. UOMS allows many core functions [e.g., micrometer scale fluidic channels, high flow rate, reversible fluidic valves, open-fluid cell/particle trapping, self-organized anisotropic extracellular microenvironments] and also novel functions including autonomously regulated oxygen microenvironments (AROM). These fundamental breakthroughs bridge the gap between open microfluidics and the classic, closed channel/chamber microfluidics and moreover, make open microfluidic devices competitive in a broad range of applications in biology and biomedicine ranging from basic to translational. Examples include the use of ELR's anti-biofouling properties to study systemic fungal dispersion/infection and to create lossless analytical systems (e.g. rare-cell diagnostics, genomic analysis, rapid antimicrobial susceptibility testing, and detection of heteroresistance). Other examples include improved systems for more in vivo-like in vitro cell culture that supports tumor microenvironments, cell migration, multispecies microbial communities, gut-microbe homeostasis, and three-dimensional neural network reintegration.

I6A.3 (Cancer) Theranostics with Radiolabeled Nanomaterials

Vilas Distinguished Achievement Professor Weibo Cai[1]
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6A | Nanomaterials and diagnostic devices, Bay Trust Forum, February 10, 2023, 10:50 AM - 12:50 PM

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 each category will be briefly illustrated in this talk, with the main focus on our own work that involves radiolabeling of various nanomaterials via “specific trapping”. The nanomaterials investigated in our laboratory include silica/carbon-based nanomaterials, DNA nanostructures, iron oxide nanoparticles, micelles, multifunctional/multimodal hybrid nanomaterials, COVID-19 nanovaccine, among others [1-6].

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6A.1 Tubular glassy carbon microneedles with fullerene-like tips for biomedical applications

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Glassy carbon, also known as “glass-like carbon” or “vitreous carbon” is an allotrope of carbon, which combines glassy and ceramic properties with those associated with graphite and has been of scientific and technological interest for over fifty years.

However, as understanding its microstructure is far from straightforward, it continues to be an area of active research. Glassy carbon adopts different allotropes depending on the hybridizations of the C–C bond, that is, sp, sp2, or sp3. Furthermore, a variety of short-range ordering effects can interact with each other and this, along with the effects of microporosity, grain boundaries, and defects, render this a fascinating material.

Glassy carbon has good electrical and thermal conductivities, excellent chemical stability, and good biocompatibility, which has led to many advanced technological applications [1]. The use of glassy carbon as an electrode material in electrochemistry is probably its best-known application.

Here, we examine the characteristics of the glassy carbon produced by catalytic pyrolysis of methane. Our results show clear experimental evidence for a fullerene-like structure. So far, evidence for this was inferred from TEM observations and theoretical models of polymer-derived carbons [2]. This work provides new insights into the structure of glassy carbons relevant to the application of glassy carbons as a biomaterial, for example, as a new form of carbon-based microneedles. Metallic needles can introduce toxic/allergenic species into susceptible subjects therefore, alternative carbon-based microneedle have great potential as replacement biomedical material for metallic needles in the field of neural engineering and as acupuncture needles.

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6A.2 Moiré superlattices in reciprocal space

Dr Maxime Le Ster[1], Dr Iaroslav Lutsyk, Mr Wojciech Ryś, Dr Paweł Dabrowski, Dr Maciej Rogala, Prof Paweł Kowalczyk
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6A | Nanomaterials and diagnostic devices, Bay Trust Forum, February 10, 2023, 10:50 AM - 12:50 PM

Moiré superlattices are ubiquitous in the study and investigation of two-dimensional (2D) materials. They emerge due to the broken (or modified) translational and rotational symmetries that exist in the otherwise uncoupled individual lattices. The consequences of the moiré superlattice on the optical and electronic properties is the subject of an increasing number of investigations [1, 2], and the most discussed emerging property is the presence of both unconventional superconductivity and Mott insulator states in twisted bilayer graphene [3, 4]. Many other moiré-enabled properties have been uncovered including ferromagnetism, moiré excitons, moiré solitons, band-flattening, moiré topological states, etc. The theory of these phenomena is under intense debate, and in this presentation, I will introduce a novel plane wave reconstruction method that explains the emergence of moiré coupling in 2D materials [5]. The new model allows to describe with a high degree of fidelity the moiré superlattices present in the scanning tunnelling microscopy images in a variety of van der Waals-bonded multilayer systems.

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6A.3 Homojunction organic thin film transistors by selective molecular doping

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6A | Nanomaterials and diagnostic devices, Bay Trust Forum, February 10, 2023, 10:50 AM - 12:50 PM

Because foldable electronics are required to have exceptionally high mechanical stability, the development of electrical components that can withstand extreme environments has become a critical task. Conventional metallic electrodes, such as copper, aluminum, silver, and gold electrodes, exhibit excellent electrical conductivity, but their rigidity and brittleness cause the device to be susceptible to interfacial delamination between device component layers. Here, we present a simple fabrication of homojunction-based completely foldable polymer thin-film transistors (PTFTs) and logic gate arrays. The selective doping of the semiconducting polymer layer enables the successful formation of a homojunction between the semiconductor and the electrode as an alternative to existing heterojunction-based devices; this homojunction consequently improves the mechanical stability of the PTFTs. In addition, work function changes (with depth) in the doped regions as induced by the sequential doping with FeCl3 promote efficient charge injection to (or from) the semiconducting region, and consequently, the contact resistance of the fabricated doped-semiconductor–based PTFTs is comparable to that of Au-electrode–based PTFTs, although the electrical conductivity and work function of the former are lower than those of the latter. In addition, the interfacial adhesion in the PTFTs was improved by interfacial cross-linking between adjacent component layers (e.g., the semiconductor/substrate and semiconductor/dielectric interfaces). The electrical performance of the resulting PTFTs was maintained without noticeable degradation even after extreme folding, suggesting that the proposed fabrication strategy can further be applied to various semiconducting polymers for the realization of foldable electronics.

6A.4 Desalination Performance of a Passive Solar-Driven Membrane Distiller: Effect of Middle Layer Material and Thickness

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6A | Nanomaterials and diagnostic devices, Bay Trust Forum, February 10, 2023, 10:50 AM - 12:50 PM

Water scarcity is a global problem, and membrane-based desalination technologies are one of the promising solutions to this problem. This study fabricated and tested a passive solar-driven membrane distiller for its desalination performance. The distiller was composed of a TiNOX plate solar absorber, cellulose-based upper and lower hydrophilic layers, a hydrophobic middle layer, and aluminum heatsinks.

The effect of the middle layer material and thickness on the desalination performance was investigated in terms of distillate productivity and salinity. The materials used for the middle layer were a screen mesh (2 mm, 4 mm, and 6 mm thickness) to generate an air gap, a PTFE membrane (0.3 mm thickness)), and a combination of the screen mesh and the PTFE membrane (2.3 mm total thickness). Salt water (35 g/L NaCl) was desalinated using the distiller at a rooftop setting at the University of San Carlos, Cebu City, Philippines.

The highest distillate productivity of 1.08 L/m2-h was achieved using a 2-mm screen mesh (air gap), but it also resulted in a high distillate salinity of 25.20 g/L. Increasing the thickness of the air gap lowered the distillate salinity but also decreased the distillate productivity. The lowest salinity of 1.07 g/L was achieved using a 6-mm air gap, but the productivity was reduced to 0.08 L/m2-h. The use of the hydrophobic PTFE membrane increased productivity (0.44 L/m2-h) compared to a 6-mm air gap but produced a distillate with high salinity (16.68 g/L). When using a combination of the screen mesh and the PTFE membrane, the productivity was 0.13 L/m2-h and a distillate salinity of 1.61 g/L.

The distiller with a thick air gap as the middle layer can deliver a distillate with low salinity and is preferred over a thin hydrophobic PTFE membrane. The use of a combination of the air gap and PTFE membrane slightly increased the productivity with comparable distillate salinity. Modifications and optimizations to the distiller can be done to improve its performance further.

I6B.1 A device-based approach to measuring the electrical conductivity of microscale metal-organic-framework (MOF) single crystals

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6B | MOFs, MOCs and cages, Skellerup, February 10, 2023, 10:50 AM - 12:50 PM

Charge transfer in redox-active metal-organic frameworks (MOFs) is of significant interest towards potential applications in electronic devices, electrocatalysis and energy storage [1]. Electrical conductivity measurements are vital to characterizing and understanding charge transfer processes arising from the underlying chemistry of novel MOFs. The small crystallite size typically obtained for novel MOFs presents a significant challenge and often forces studies using pressed powder pellets rather than individual single crystals.

In a pressed pellet measurement, the interfaces between crystallites add significant resistance and can contribute non-linearity to the current-voltage characteristics. Pressed pellet measurements are also intrinsically isotropic because relative crystallite orientation is random, hiding any anisotropy that might exist at single crystal level. The pressure applied to form the pellet can cause crystallite damage and built-in strain that may further affect the measured conductivity. This makes single crystal measurements more desirable, but they are also rare due to the challenges involved. The dominant route to single-crystal MOF conductivity measurements presently are the ultra-sharp probe approaches demonstrated by Sun et al. [2], however these are remarkably intricate and best suited to needle-like morphologies.

We explored MOFs based on the bis-[1,2,5]-thiadiazolo-tetracyanoquinodimethane (BTDAT) molecule due to its delocalized structure and strong electron accepting properties, in particular, the 2D framework [Cu(BTDAT)(MeOH)], which we recently synthesized [3]. This MOF can be obtained as single crystals in a platelet-like morphology with a size of order 10-100 microns. Given this morphology, we developed an new approach to electrical measurements of single-crystal MOFs that uses a thin pre-patterned polydimethylsiloxane layer on a silicon wafer [4,5]. Notably, this approach gives the ability to 'break and remake' contacts to study electrical conductivity as a function of crystal orientation. It also has the potential for development of MOF-based field-effect transistors (MOFFETs). We use this approach to show that [Cu(BTDAT)(MeOH)] single crystals have semiconducting behaviour with a typical conductivity of 40 uS/cm and high in-plane directional conduction isotropy.

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I6B.2 Operando Infrared and Nuclear Magnetic Resonance Methodologies for Probing Chemistry of Working Batteries

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6B | MOFs, MOCs and cages, Skellerup, February 10, 2023, 10:50 AM - 12:50 PM

Developing robust and informative operando characterization methodologies to advance our fundamental understanding of metal-ion rechargeable battery chemistry under real or quasi-real working condition is highly desirable but much of it is still in early stage.[1,2] In this presentation, we will discuss two patented operando methodologies: dual-IR window/electrode attenuated total reflection (ATR) infrared spectroscopy[3] and strip-line nuclear magnetic resonance spectroscopy.[4] In both methodologies, the cell configuration is real-world battery-like, i.e., the electrodes, electrolyte and separator are in lamellar arrangement and their thickness and distance in micrometer scale. We will present proof-of-concept cases demonstrating that the investigative power of IR and NMR are largely retained and the methodologies are overall robust.

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I6B.3 Metal-organic cage assemblies for gel engineering

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6B | MOFs, MOCs and cages, Skellerup, February 10, 2023, 10:50 AM - 12:50 PM

A gel is a soft material containing a cross-linked three-dimensional network and a continuous phase like a liquid. Most gel materials reported so far are composed of cross-linked organic polymers or silica-based networks. Recently metal-organic network systems started contributing to this class of materials. In this case, either amorphous metal-organic networks or colloidal networks based on metal-organic frameworks (MOFs) are used; however, it has been challenging to control their cross-linked network structures. Our group recently reported another type of metal-organic network to form gels, in which well-defined metal-organic cages (MOCs) are used as building blocks and their inter-cage linkage is tuned by coordination chemistry. This network further produces colloidal spheres, followed by connecting them to form colloidal networks.[1,2] This hierarchical nature of metal-organic networks based on MOCs gives us an opportunity to control their cross-linked networks across multiple length scales.[3,4] In this presentation, we will discuss the strategies to regulate the cross-linked networks of MOCs and tune the resulting properties including porosity.

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6B.1 Novel hierarchical copper-based metal-organic frameworks for improved catalytic performance

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6B | MOFs, MOCs and cages, Skellerup, February 10, 2023, 10:50 AM - 12:50 PM

Introducing additional meso- or macroporosity into traditionally microporous metal-organic frameworks (MOFs) is a very promising way to improve the catalytic performance of these materials, mostly due to the resultant reductions of diffusional barriers during liquid-phase or gas-phase reactions. Here we show that HKUST-1 can be successfully synthesised either via post-synthetic treatment (etching prepared HKUST-1 samples in phosphoric acid) or via in situ crystallisation (exposing the MOF precursor solution to supercritical CO2) to produce hierarchically porous structures that are highly beneficial for catalysis. These hierarchical MOFs were characterised by PXRD, SEM and gas sorption to confirm the preservation of the microscopic structure and the appearance of macropores in the crystallites. More importantly, the benefits of introducing these hierarchical porous structures into this MOF for improving the diffusion accessibility of reagents to the sample in catalysed liquid- and gas-phase reactions were quantified for the first time. It was found that the hierarchical pore structure helped to increase the reaction conversion of styrene oxide methanolysis (by ~65 % using either HKUST AE and HKUST CO2, at 40 oC in 25 min) and CO oxidation (by ~55 % using HKUST CO2 at 260 oC). These findings demonstrate the advantage of using hierarchical porous MOFs in catalysis.

6B.2 Robust organic cages from cavitands: construction and cargo logistics

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6B | MOFs, MOCs and cages, Skellerup, February 10, 2023, 10:50 AM - 12:50 PM

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 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 incarcerated or can be exchanged for solvent.

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6B.3 Using metal complexes to open the door to long-lived excited states

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6B | MOFs, MOCs and cages, Skellerup, February 10, 2023, 10:50 AM - 12:50 PM

Creating long-lived excited states that have the potential to act as catalytic centres is an important research goal. One way to achieve this is to use metal complexes in which the ligand has a triplet charge-transfer (3ILCT) state that can easily be accessed because of the presence of the metal centre. A number of these systems have been reported based on rhenium(I) with polypyridyl ligands. The complexity of the photophysics of these systems is challenging in terms of designing compounds. For example, we have recently demonstrated that solvent effects can tune between differing excited states1 and that modest peripheral changes to compounds can result in dramatic changes in excited state lifetime2.
Rhenium(I) and ruthenium(II) complexes with polypyridyl ligands with donor group ((triphenylamine, TPA) can have long-lived excited states. We report how these can be Characterised and what design features we can learn from these studies. The challenge of using earth abundant metals to achieve these same types of states will also be introduced

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6B.4 MOFs for CO2 Electroreduction

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6B | MOFs, MOCs and cages, Skellerup, February 10, 2023, 10:50 AM - 12:50 PM

Carbon emissions are at an all-time high with global efforts being explored to reduce the effect of these emissions on the globe. Carbon reduction methods are of particular interest as it can actively reduce CO2 back into useful materials. This requires the addition of a catalyst to facilitate the amount of energy used in the reduction process.

An electrocatalyst is used in electrochemical processes where electricity is used to facilitate the reduction process. An ideal electrocatalyst will contain multiple catalytic sites which contribute to the selectivity and turn over frequency of catalytic reactions. For this reason, metal-organic frameworks (MOFs) have obtained interest in the application of electrocatalysis.[1] The interest arises from innate features of MOFs including high surface areas, versatility and dispersion of catalytic sites. However, the electrocatalytic reduction of CO2 in MOFs are greatly limited by two factors. These include mass transport of CO2 to catalytic sites and low electrical conductivity of MOFs.

This research explores techniques to improve these two limiting factors which have not been widely investigated. Mass transport can be greatly increased by using a gas diffusion cell (GDC) to conduct the electrochemical reactions rather than using the standard H-cell setup.[2] This setup is not limited by the solubility of CO2 in solution as it uses a constant flow of gas therefore increasing mass transport to the electrocatalyst.[3] The electrical conductivity of MOFs can be increased by utilising the pores to grow conductive polymers.[4] The results will unlock the great potential for MOFs in the field of electrocatalysis.

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I6C.1 What happens when you make a quantum well antiferromagnetic?

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6C | Condensed-matter theory, WSP, February 10, 2023, 10:50 AM - 12:50 PM

Unlike their ferromagnetic cousins, antiferromagnetic materials had long been considered to be essentially useless like paramagnets [1] – until the concept of antiferromagnetic spintronics emerged recently [2]. Since then, the interplay between antiferromagnetic order and electronic properties has become an active area of research, focusing on interesting fundamental-science questions and exploring potential spintronics applications [3]. We add an intriguing new dimension to this research field by comprehensively answering the question posed in the title [4].

Quantum wells are textbook examples for illustrating the effect of a confinement potential on quantum particles. They are also routinely realised in semiconductor heterostructures such as AlGaAs/GaAs/AlGaAs, where the larger band-gap size in the barrier material (AlGaAs) confines charge carriers to two-dimensional bound states in a thin layer (GaAs). We consider the situation where the bulk materials used to create the quantum well are diamond antiferromagnets. We find that the antiferromagnetism in the crystals gives rise to antiferromagnetic order of the quasi-2D charge carriers that is signified by a quadrupolar equilibrium-current distribution. We derive an envelope-function theory for the diamond-antiferromagnet band structure and use it to define a quantity that describes collinear orbital antiferromagnetic order of the band electrons, in the same way a magnetization signals ferromagnetic order. An electric field applied perpendicularly to the plane distorts the quadrupolar equilibrium-current distribution of quasi-2D charge carries, inducing a dipolar current associated with a magnetisation. We obtain a complete theoretical description of such magnetoelectric effects based on the underlying antiferromagnetic order of quasi-2D carriers and discuss applications.

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I6C.2 Electrically-induced spin torques due to the bulk states of topological insulators

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6C | Condensed-matter theory, WSP, February 10, 2023, 10:50 AM - 12:50 PM

The last decade has witnessed tremendous interest in spin-orbit torques (SOT), which offer an all-electrical way to control magnetization dynamics, thereby enabling faster, more efficient operation of magnetic memory and computing devices. Spin-orbit torques are especially strong in topological materials, such as topological insulators and Weyl and Dirac semi-metals, because most of them break inversion symmetry and have strong spin-orbit coupling. The largest spin torques to date have been observed at topological insulator/ferromagnet (TI/FM) interfaces, including room-temperature magnetization switching. However, the relative contributions of bulk and surface states to the spin torque at topological insulator (TI)/ferromagnet interfaces are poorly understood.

In this talk I will discuss spin torques due to TI bulk states. I will first review the status of the field. Topological insulator spin torques are believed to be driven by the Rashba-Edelstein effect (REE) in the surface states, the spin Hall effect (SHE) in the bulk and the magnetization penetrating a short distance into the TI. The extent to which each mechanism contributes is yet to be conclusively determined. It is believed that the bulk makes a strong contribution to the SOT, and this is customarily attributed to the spin-Hall effect. The most important unanswered questions are: how large are bulk spin torques, what types of torques are present, and how can we distinguish bulk from surface state torques?

Next I will show that: (i) There can be no spin-Hall effect in the bulk in the absence of the magnetization. In real samples the magnetization decays very quickly away from the interface, casting considerable doubt on the picture of a bulk spin-Hall effect giving rise to a spin torque at the interface; (ii) There is no spin torque coming from the bulk, even when the states interact with a homogeneous magnetization; (iii) For an inhomogeneous magnetization the spin torque depends on the magnetization gradient; its size is 1 - 2 orders of magnitude smaller than the surface state contribution for the gradients at which our theory is valid, though we argue that it may compete with the surface state contribution at the much larger gradients expected in experimental samples; (iv) In stark contrast to the 2D case, the size of the torque on the out-of-plane magnetization is comparable to that on the in-plane magnetization, which can be considered an experimental smoking gun for the bulk contribution, should it prove to be significant.

I6C.3 A natural surprise: The superconductivity of Rh17S15

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6C | Condensed-matter theory, WSP, February 10, 2023, 10:50 AM - 12:50 PM

Despite the large variety of different mineral compounds found in the earth's crust, most materials of interest in solid state physics are artificial, i.e. only produced in the lab. Apart from native metals such as tin or lead, naturally-occurring superconducting compounds are rare. One of only a handful of such materials is the cubic mineral $Rh_{17}S_{15}$, also known as miassite, which can be found near the Miass River in the southern Urals of Russia. Although the first observation of superconductivity in laboratory-grown $Rh_{17}S_{15}$ was reported almost 7 decades ago [1], this material has attracted renewed interest in the last 15 years as a strongly-correlated superconductor. In particular, both the heat capacity jump at the critical temperature and the upper critical field significantly exceed theoretical expectations [2]. Nevertheless, the key microscopic parameter governing the superconductivity – the superconducting gap – has remained unclear. In this talk I will outline our work to determine this quantity through penetration depth and controlled disorder experiments [3]. The consistent picture emerging from our results evidences a surprisingly unconventional pairing state, revealing $Rh_{17}S_{15}$ to be a naturally unique superconductor.

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6C.1 Quantum transport in a background medium: Fluctuations versus correlations

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6C | Condensed-matter theory, WSP, February 10, 2023, 10:50 AM - 12:50 PM

Charge transport normally takes place in some background medium. To understand how the environment affects the moving carrier and vice versa is a difficult question and in this generality at present perhaps one of the most heavily debated issues in condensed matter physics. We propose a two-channel transport model that captures this interplay by means of a novel fermion-boson coupling in an effective way. The model is analysed in the one-particle sector by exactly calculating the optical conductivity, Drude weight, quasiparticle dispersion and particle-boson correlation functions for a 1D infinite system. Connections to the transport of lattice and spin polarons were established. For the half-filled band case, we determine numerically the groundstate phase diagram and prove that the model exibits a metal-insulator quantum phase transition. The behaviour of the Luttinger liquid charge exponent, the charge excitation gap, the momentum distribution function and the photoemmission spectra show that the metallic phase typifies a repulsive Luttinger liquid, while the insulating phase constitutes a charge density wave. The results are related to the more standard Mott and Peierls transition scenarios.

6C.2 Using nano-electronics as a tool in materials science: unravelling the mystery of two-level defects in amorphous solids

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6C | Condensed-matter theory, WSP, February 10, 2023, 10:50 AM - 12:50 PM

Superconducting electronics are one of the best understood and most promising platforms for realising quantum information processing. Unfortunately they suffer from the presence of defects comprised of uncontrolled two-level systems, which reside in the materials used to construct them. These defects can lead to low of energy, coherence and imperfect control pulses.

Interestingly, this observation is directly related to a much older and well-known problem from solid-state physics; what is the origin of the two-level defects thought to dominate the behaviour of amorphous glasses at very low temperatures? At present the precise microscopic origin of these defects remains a mystery, but recent work both experimental and theoretical, is bringing us closer to an answer.

Using superconducting qubits as probes of metallic oxide thin films has opened up new opportunities to study individual two-level defects. New experiments have surveyed and characterised individual defects, as well as studying their electric field, temperature and strain dependence. Direct coupling between individual defects has also been measured for the first time. The next generation of experiments combined these ideas with acoustic probes of defect dynamics, neutron scattering experiments and even probes of cosmic ray flux.

In this way, new information is being obtain about defects in amorphous materials which not only improves low temperature electronics, but also increases our understanding of this critically important phase of matter.

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6C.3 "topotronics" with 2D-Xenes - from quantum matter to emerging devices

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6C | Condensed-matter theory, WSP, February 10, 2023, 10:50 AM - 12:50 PM

We present two novel “topo-tronic” device constructs using topological phases in 2D-Xenes: (i) a robust topological valley filter [1], and (ii) a topological quantum field effect transistor [2] aimed at overcoming the “Boltzmann tyranny”.

First, we present a realizable device design for an all-electrical robust topological valley filter [1] that utilizes spin protected topological interface states hosted on monolayer 2D-Xene materials with large intrinsic spin-orbit coupling. Using quantum transport simulations, we confirm the role of spin-orbit coupling in achieving an improved valley filter performance with a perfect quantum of conductance attributed to the topologically protected interface states. Our analysis further elaborates clearly the right choice of material, device geometry and other factors that need to be considered while designing an optimized valleytronic filter device [1].

Next, we propose a topological quantum field-effect transistor (TQFET) that be engineered to enable sub-thermionic transistor operation coupled with dissipationless ON-state conduction. Detailing the complex band translation physics related to the quantum spin Hall effect phase transition, It is the demonstrated transitions between the quantum spin-valley Hall (QSVH) and the spin quantum anomalous Hall (SQAH) phase can ultimately ensure the topological robustness of the ON state while surpassing the thermionic limit.

We finally comment on other systems like superconducting hybrid systems that rely on Rashba spin-orbit coupling for advanced device functionalities and also a peek into our current ventures on understanding dephasing across topological channels [3].

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6C.4 Topological-Insulator Nanocylinders

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6C | Condensed-matter theory, WSP, February 10, 2023, 10:50 AM - 12:50 PM

Nanostructures, such a quantum dots or nanoparticles, made of three-dimensional topological insulators (3DTIs)[1-5] have been recently attracting increasing interest, especially for their optical properties.
We present results for the energy spectrum, the surface states and the dipole matrix elements for optical transitions with in-plane polarization of 3DTI nanocylinders of finite height *L* and radius *R*. We first derive an effective 2D Hamiltonian by exploiting the cylindrical symmetry of the problem. We develop two approaches: The first one is an exact numerical tight-binding model obtained by discretising the Hamiltonian; The second one, which allows us to obtain analytical results, is an approximated model based on a large-*R* expansion and on an effective boundary condition to account for the finite height of the nanocylinder.

We find that the agreement between the two models, as far as eigenenergies and eigenfunctions are concerned, is excellent for the lowest absolute value of the longitudinal component of the angular momentum.

Finally, we derive analytical expressions for the dipole matrix elements by first considering the lateral surface alone and the bases alone, and then for the whole nanocylinder.

In particular, we focus on the two limiting cases of tall and squat nanocylinders. The latter case is compared with the numerical results finding a good agreement.

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I6D.1 Perylene derivatives for polariton lasing

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6D | Optical materials and extreme environments, Downer, February 10, 2023, 10:50 AM - 12:50 PM

Strong coupling in organic media holds the promise of efficient room temperature polariton lasing with solution-processed materials. Currently, however, only a handful of pure organic materials have been shown to demonstrate polariton lasing. A major challenge is to achieve high exciton-photon coupling while maintaining high photoluminescence quantum yield.

Here, I will discuss our recent work on using perylene materials to demonstrate optically pumped lasing. We utilize a series of perylene diimide materials that possess sterically hindered substituents, dispersed within a polymer matrix. The rigid structures prevent aggregation and allow high photoluminescence quantum yields (PLQYS) at large dye loadings. We demonstrate that these systems can exhibit Rabi splittings up to 150 meV with PLQYs of > 70%, [1] and polariton lasing evidenced by threshold behavior, strong directionality, and slight blueshifting of organic polariton systems. [2]

We expect that continuous exploration of new dyes will allow improved performance and low power requirement in organic semiconductor lasing.

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I6D.2 Engineering Scalable Electrocatalysts for Affordable Production of Green Hydrogen

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6D | Optical materials and extreme environments, Downer, February 10, 2023, 10:50 AM - 12:50 PM

Protecting our planet while sustaining industrial and economic growth is an ambitious and essential aim that needs to be achieved at a global scale to be successful. Governments have expressed worldwide support to commit to net-zero emission targets to mitigate climate change. This requires development of new technologies to rapidly decrease our reliance on fossil-fuel resources. Chemical storage of renewable energy harvested from solar farms and wind by electrochemical hydrogen production is an attractive approach to enable the export of renewable energy to countries with less access to renewable energy sources and/or very high population density. Electrochemical hydrogen production is also beneficial as an intermediary large scale energy storage approach for stabilization of the electrical grid and on-demand off-the-grid power generation. While a variety of carbon-emission-free electrochemical hydrogen production technologies have reached commercial maturity, they still rely on rare and expensive electrocatalyst that undermines their inherent scalability below that required for adoption of hydrogen as global energy carrier. Furthermore, the high cost and poor lifetime of these rare catalysts increase the cost electrochemical production of hydrogen hindering its economic sustainability.

In this paper, we will discuss emerging approaches for the use of low-cost earth abundant materials as efficient electrocatalysts for green hydrogen and e-fuels production. The multi-scale engineering of nano-micro materials and their integration in effective macro-scale morphologies will be presented as successful strategy for the use of a variety of earth-abundant rock forming elements as electrodes and membranes of electrolysers. The need to overcome the limitations imposed by single constituent such as the poor electrical conductivity of iron oxide and/or surface activity of manganese oxide will be demonstrated by the fabrication of highly performing nano-micro composite electrocatalysts made of carefully controlled hierarchical structures. We will showcase the use of the latest generation of flame-aerosol synthesis reactors for the direct roll-to-roll fabrication of electrodes for alkaline and acidic electrolysers, demonstrating a scalable path for the low-cost production of green hydrogen from renewable energy sources. The advantages and challenges of the flame synthesis route will be critically discussed providing directions for its optimization as a scalable technology for electrocatalyst production.

I6D.3 Plasmonic and dielectric nanostructures for enhanced light harvesting, emission control, and nanometrology

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6D | Optical materials and extreme environments, Downer, February 10, 2023, 10:50 AM - 12:50 PM

The first part of my talk focuses on disordered arrays of plasmonic colloids that enable broadband optical absorption. This is due to equipartition of energy and convergence of internal mode lifetimes. The optical response can be tuned via coupling to an underlying Fabry-Perot cavity, enabling narrow reflection suitable for color generation [1]. Surprisingly, the far-field properties, i.e. the perceived color in reflection, is independent of the colloidal material [2], with potential applications in solar light harvesting for energy conversion and photocatalysis. Due to reciprocity, such disordered surfaces can also be used to enhance light extraction from underlying high-index dielectric layers, via simple deposition of the disordered array on for example commercial GaN LEDs [3].

In the second part I will present recent research on dielectric metasurfaces for control of non-linear emission of low-dimensional materials deposited on top. Particularly we developed a spatially compact design for obtaining sharp optical resonances via bound states in the continuum (BIC), a radial-BIC consisting of ring-like arrangement of dielectric resonators [4]. This system is ideally suited for interfacing with flakes of two-dimensional monolayers. We further show how the chiroptic response of monolayer halide perovskites can be enhanced via coupling with chiral dielectric metasurfaces [5].

The talk will finish with an intriguing application of plasmonic nanoparticles in metrology, namely the in-situ assessment of oxygen vacancies lifetimes in metal oxides, based on photo-induced enhanced Raman scattering [6-8]. Here, the properties of UV-generated vacancies are interrogated via their influence on the Raman scattering enhancement of metallic colloids.

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8. Glass et al, ACS Energy Letters 6, 4273 (2021)

6D.1 Photo-triggered Charge Transfer of 2D-TMD-based Heterostructures: Implications in Exciton Optoelectronics

Professor Jinsoo Joo[1], Dr. Jun Young Kim[1], Sang-hun Lee[1], Professor Jeongyong Kim[2]
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6D | Optical materials and extreme environments, Downer, February 10, 2023, 10:50 AM - 12:50 PM

Heterostructures (HSs) using two-dimensional transition metal dichalcogenides (TMDs), perovskites, organic semiconductors, and quantum-dots (QDs) are promising platforms for advanced exciton optoelectronics. Hetero interlayer excitons (HIXs) of the HS of monolayer WS_2 and multilayer PbI_2 were investigated (3 - 293 K). The drastic decrease in PL intensity of the WS_2/PbI_2 HS indicates the occurrence of charge transfer. PL peaks corresponding to neutral excitons, trions, and biexcitons of WS_2 were observed in the HS. Notably, intense PL emission due to HIXs in the HS was observed in visible light region at 675-700 nm. With increasing excitation power, PL peaks of HIXs in the HS were blue-shifted, originating from the screening effect of Coulomb repulsive interaction between dipole-aligned HIXs. The lifetime of HIXs from time-resolved PL spectra at 3 K was 8.6 times longer than that of intralayer excitons.[1]

Field-effect-transistors (FETs) using n-type MoS_2 and p-type organic rubrene HS exhibited anti-ambipolar transistor characteristics with the coexistence of n-, p-, and off-states controlled by gate bias. The photo-triggered FETs using MoS_2/rubrene HS were operated by light irradiation without applying source-drain bias. Distinctive ternary inverters employing MoS_2/rubrene FETs were improved through incident light.[2]

For the HSs of $MoSe_2$ and WSe_2 with perovskite $CsPbX_3$ (X=Br, Cl, I)-QDs, PL quenching of the QDs was observed owing to charge transfer. Upon light irradiation, n-channel current in both $MoSe_2/CsPb(Cl/Br)_3$-QDs and $WSe_2/CsPbBr_2I_1$-QDs FETs increased, and V(th) was negatively shifted owing to photogating effect induced by trapped holes. The photoresponsivities of the FETs increased with the QDs, suggesting application in photodetectors.[3]

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6D.2 Metafibre Optics: Principles, Fabrication, and Applications

Dr Haoran Ren[1], Mr Jaehyuck Jang[2], Mr Chenhao Li[3], Mr Andreas Aigner[3], Dr Malte Plidschun[4,5], Mr Jisoo Kim[4,5], Prof. Junsuk Rho[2,6,7], Prof. Markus A. Schmidt[4,5,8], Prof. Stefan A. Maier[1,3,9]

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6D | Optical materials and extreme environments, Downer, February 10, 2023, 10:50 AM - 12:50 PM

The development of ultracompact, flexible, and versatile fibre-based technology for advanced imaging has the potential for a profound impact on many photonic, biological, and medical applications. Meta-optics, which allows complete wavefront control of light by ultrathin subwavelength structures, has offered a transformative platform for both fundamental study of light–matter interactions at a nanoscale and a diverse range of photonic applications. In this presentation, I will introduce our recent work in 3D metafibre optics with unleashed height degree of freedom for all-on-fibre wavefront manipulation [1, 2].

We fabricated a 3D achromatic diffractive metalens on the end face of a single-mode fiber, achieving achromatic and polarization-insensitive focusing across the entire near-infrared telecommunication wavelength band ranging from 1.25 to 1.65 μm [2]. The unlocked height degree of freedom in 3D nanopillar meta-atoms largely increases the upper bound of the time-bandwidth product of an achromatic metalens, leading to a wide group delay modulation range and thereby a broad wavelength coverage. Furthermore, we demonstrate the use of our compact and flexible achromatic metafiber for fiber-optic confocal imaging, capable of creating in-focus sharp images under broadband light illumination. I will finish my talk by presenting our recent development of vectorial metafibers for the generation of arbitrary structured vector beams on a high-order Poincaré sphere, including those carrying different orbital angular momentum modes.

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6D.3 Plasmon-enhanced optical properties of molecular chromophores coupled with size-tuned silver nanoparticles

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6D | Optical materials and extreme environments, Downer, February 10, 2023, 10:50 AM - 12:50 PM

Plasmonic silver nanoparticles offer a highly tunable platform for modulating the optical properties of nearby chromophores.[1–3] In order to understand the detailed mechanism of chromophore-nanoparticle interactions it is important that the silver particles have well-controlled and narrowly distributed morphologies and their coupling distances can be precisely controlled.[4] In this seminar we describe an optimised silver nanorod synthesis and purification procedure that can produce nanoparticles with low size and shape distributions. The optical absorbance and scattering properties of these particles can be tuned across the visible to near-IR spectral window. These nanoparticles are then used to fabricated monolayer films to engineer controllable coupling with over-layered chromophores. We demonstrate the enhancement of chromophore absorption and fluorescence using nanorods that are specifically tuned to molecular resonances, and offer insight into the factors that control the coupling of plasmon and chromophore transitions. Ultimately, these systems will be used to increase efficiency in light-harvesting or photo-emission applications.

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I6E.1 Protein Assemblies at Interfaces: Fundamentals and Opportunities

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6E | Bio 6 – proteins, diagnostics and devices, Sigma, February 10, 2023, 10:50 AM - 12:50 PM

Self-assembling protein subunits that form hollow cage-like structures, called protein cages, have been investigated as potential molecular carriers. However, tuning the release rate of encapsulated molecules from these protein cages is a challenge. We hypothesize that by rationally modulating the protein-protein interactions between the protein cage subunits, the release of molecular cargo from the lumen can be tuned. To test the hypothesis, we introduced modifications at the intersubunit interface and the interaction surfaces between two molecules by introducing non-native histidines or substituting the interacting surfaces with other peptide sequences. The effects of the modifications were characterized at various pH-s. The results show that rational modifications of protein-protein interactions have implications on the self-assembly and hence, release rate of the encapsulated molecules.

In recent studies, we found that these protein cages form an ensemble that stabilize oil droplets in water by localizing at the oil-water interface and forming Pickering emulsion. However, their behavior and structural integrity at this interface is rarely studied. Our works elucidate the unique behavior of the protein nanocages that is distinct from other small (monomeric/dimeric) proteins. The protein cage-stabilized emulsion is pH-responsive.

In conclusion, protein cages can serve as an individual molecular carrier or as an ensemble that stabilizes an emulsion and present many opportunities that are yet to be explored.

I6E.2 Amyloid fibril proteins: health, disease and applications

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6E | Bio 6 – proteins, diagnostics and devices, Sigma, February 10, 2023, 10:50 AM - 12:50 PM

Amyloid fibrils are specific protein structures that can be formed by a range of different proteins. Amyloid fibrils were first known as hallmarks of diseases such as Alzheimer's disease, where proteins change from their normal functional fold, and aggregate into non-functional amyloid fibrils that form large deposits. More recently, it has been found that amyloid fibrils carry out important functions in a range of organisms, including coating surfaces of fungal spores and providing "switches" in human cellular signalling pathways. Furthermore, the unusual properties of some amyloid fibrils have led to applications of these proteins in various biotechnological fields. In this presentation I will discuss two amyloid proteins: one functional amyloid from fungi and once human cancer-related protein. Hydrophobins are fungal proteins that convert to amyloid fibrils at interfaces and create protective coatings on fungal spores. The amphipathic layers that these fibrils form are extremely stable and therefore many applications have been proposed. Secondly, the human protein p16 is a tumour suppressor that is mutated in many cancers. We have discovered that under oxidizing conditions, the protein reacts through its single cysteine residue to form dimers that then self-assemble into amyloid fibrils. This fibril formation is completely reversible, and therefore the cysteine reactivity acts as a switch between the two structural states, making p16 an excellent model to study amyloid fibril formation. We are currently investigating the structure and formation mechanism of p16 amyloid fibrils, using a range of approaches. These findings will give insight into a novel disulfide-linked amyloid structure.

I6E.3 Coevolution-driven and likelihood-based design of proteins for industrial applications.

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6E | Bio 6 – proteins, diagnostics and devices, Sigma, February 10, 2023, 10:50 AM - 12:50 PM

The harsh conditions of industrial workflows are often incompatible with the physiological micro-environments in which proteins evolved, making the utilisation of proteins in industrial setups, challenging. Protein resilience is however more generally coded in their three-dimensional structure, the acquisition of which results from billions of years of protein evolution.

Through a computational workflow starting from the co-evolutionary information found in protein sequences that share the same ancestry, we aim to increase protein stability by stabilising their fold. We attempt this with a combination of computational approaches working orthogonally in both protein sequence and structural spaces. Via Monte-Carlo simulations instructed by co-evolutionary information we generate random sequences that we test firstly in-silico via high-temperature structure-based molecular dynamics simulations and then experimentally validate.

This reduces the search of viable sequences within the enormously large protein sequence space, overcomes problems of patentability by quickly differentiating new designs from the sequence of a template protein, and reduces to a minimum the experimental efforts and costs needed to validate otherwise large amounts of potential candidates.

To show the effectiveness of the method, I will present the recent design of new protein inhibitors with consistently increased melting temperatures.

Overall, the generalisability of this approach creates a unique opportunity to design novel and robust functional proteins, ultimately widening their applicability in industry.

6E.1 Measurement of Cell Motility using Differential Dynamic Microscopy (DDM)

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6E | Bio 6 – proteins, diagnostics and devices, Sigma, February 10, 2023, 10:50 AM - 12:50 PM

The ability of cells to explore their environment is important for a range of biological systems, including bacteria, algae, and spermatozoa. The independent motion of cells is known as cell motility, and allows for cells to seek out nutrients, follow chemical signals and propogate1. There are a wide range of motilities including swimming, swarming, twitch-gliding, and sliding2,3. Movement can be realised through the manipulation of flagella or the reduction of pili, as evidenced in systematically separated phyla3. The classic example is the swimming 'run and tumble' motility of Escherichia coli (E. coli). Standard methods of measuring motility involve microscopic tracking of individual cells, so only a finite number of cells can be tracked, and obtaining statistically reliable measurements of populations is time consuming and difficult.

Differential Dynamic Microscopy (DDM)4 is a relatively new technique which uses a dynamic light scattering formalism to measure the dynamics of suspended particles using a standard microscope. Videos are recorded at moderate frame rates, and fluctuations in pixel intensity are used to calculate correlation functions. As it is not necessary to resolve individual particles, measurements can be made using low magnifications and wide fields of view, providing ensemble measurements of the dynamics on up to tens of thousands of scattering objects. Since it was first applied to bacteria5-6, the technique has been applied to a range of motile systems (reviewed by Al-Shahrani and Bryant7) but has not yet reached the wider research community.

We will explain the principles of DDM, illustrates with examples of the characterization of bacterial motility, and discuss the advantages and disadvantages of the technique.

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6E.2 A transparent platform for cell capture and single cell isolation

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6E | Bio 6 – proteins, diagnostics and devices, Sigma, February 10, 2023, 10:50 AM - 12:50 PM

The recognition of cellular heterogeneity has triggered the need to develop single cell isolation and analysis techniques, so the information for each single cell, rather than the whole population was obtained, which has high significance in various aspects of biological research.[1] However, selective isolation of individual target cells from a heterogeneous population is technically challenging. In this presentation, a new platform based on a transparent semiconducting electrode for isolating individual cells from complex biological samples will be introduced.[2] The strategy to recover single cells is using a concept 'light activate electrochemistry' (LAE) which makes use of the photo-responsive property of semiconducting material.[3] To achieve the function of this new platform, one of the key element is the electrode which has Au disks of micron dimension on amorphous silicon–indium tin oxide films. Such an electrode is able to perform LAE as well as being compatible with high-resolution fluorescence microscopy.[4] The second key element of this new platform is the surface chemistry which functionalizes the patterned electrode with monolayers of different functionalities. This allows target cells to be selectively captured on the Au disks by the targeting molecules. The co-stimulation of the platform using light from a microscope and an electric potential triggers the cleavage of cell binding molecules from the Au disks to release the single cells of interest from the illuminated regions only. Using circulating tumour cells as a model, we demonstrate single cancer cells with low expression of epithelial cell adhesion molecules can be isolated from a blood mixture.[2]

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6E.3 Real-time monitoring of cancer cell metastasis in mice using lanthanide nanoparticles

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6E | Bio 6 – proteins, diagnostics and devices, Sigma, February 10, 2023, 10:50 AM - 12:50 PM

Metastasis is the main cause of cancer deaths. Despite the multistep process of so-called "metastasis cascade" has been conceptualised [1], the complex pathogenetic mechanisms remain elusive, largely due to the lack of proper in vivo imaging tools that can provide high spatio-temporal resolution for large sample areas. To shed new light on cancer metastasis, we employ lanthanide nanoparticles emitting fluorescence in the shortwave infrared (SWIR) region [2], to visualise and track cancer cells migrating in live mice. Compared to visible and near-infrared fluorescence, SWIR fluorescence penetrates 10–100 times deeper under mammalian tissues thanks to reduced absorption, scattering, and autofluorescence background, offering significantly enhanced contrast and resolution for in vivo imaging [3]. Accordingly we have developed a SWIR imaging platform incorporating motorized sample stage and zooming lens, which enables rapid surveillance of an entire mouse (~10 cm) followed by pinpointing of single cells (~10 µm), all via remote control. We use Yb/Er nanoparticles to label the cancer cells, and Nd/Er ones to display the blood vessels: while both emit SWIR fluorescence at 1525 µm, the former requires 980 nm excitation and the latter under 808 nm excitation. By multiplexing these two SWIR channels, we can unambiguously identify extravasation and seeding of cancer cells as they migrate to distant organs during blood circulation. We are currently studying the major cancer types leading to brain metastasis, including lung cancer, breast cancer, and melanoma, with the results expected to answer key questions about how diverse types of metastases arise and differentiate.

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6E.4 Sustainable electronics with carbon nanofibres for flexible sensor applications

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6E | Bio 6 – proteins, diagnostics and devices, Sigma, February 10, 2023, 10:50 AM - 12:50 PM

Existing electronics technologies based on metals (e.g. silver and gold) are expensive, non-renewable, require complex handling and carry a high environmental cost at end of life [1,2]. There are clear environmental and socioeconomic requirements to introduce more sustainable electronic components to support the reduction of environmental impact and manufacturing cost. Although graphene and carbon nanotubes (CNTs) have exhibited exceptional functionalities for applications in electronics [2], carbon sources from nature, such as lignin, a major by-product of the papermaking industry, are more sustainable and cheaper carbon precursor options [3]. In this project, we used electrospinning to fabricate lignin nanofibres and then carbonised them to form conductive carbon nanofibres. These carbon nanofibres were formulated into fully bio-based carbon inks, with amyloid protein nanofibrils added to help the dispersion of fibres and to improve their adhesion to the substrate during printing [4]. The use of water as the carrier medium for the ink also significantly reduces the fabrication cost and environmental impact. The inks were printed on flexible paper substrate, and the electrical properties of the printed carbon layer under deformation were further characterised. Carbon nanofibres are the promising material candidate for sensing applications due to their large surface area [5]. Here, we also demonstrate the use of these sustainable printed electronics for wireless moisture and strain sensor applications. By using more sustainable materials in flexible electronics, these devices can become “greener” for low cost and short life internet-of-things (IoTs) applications such as smart packaging and healthcare monitoring.

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Pl.06 The physics of quantum processors: making machines at the atomic-limit

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Plenary Session 6, Bay Trust Forum, February 10, 2023, 1:50 PM - 2:40 PM

Sixty years ago, in 1960, the great American physicist Richard Feynman delivered a famous lecture in which he urged experimentalists to push for the creation of new materials with features designed at the atomic limit. He called this the “final question”: whether ultimately “we can arrange the atoms the way we want: the very atoms all the way down!"

This session will describe how we are now finally delivering on Feynman’s dream. I will explain how to manufacture materials and devices whose properties are determined by the placement of individual atoms, and I will highlight the creative explosion in new devices that has followed and the many new insights into the quantum world that this revolution has made possible.

Poster Session 1

Poster	Presenting Author Names	Poster Title
P1.001	Dr Saeedeh Afsar	ATR-FTIR spectroscopy and chemometric analyses of bumble bee secretions from hungry queens and workers
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P1.121	Miss Maria Zafar	Shelf life enhancement of agricultural products via coating of simply synthesized nanoparticles
P1.122	Amira Ramadan Alghamdi	Materials Intermixing and the Dipole Formation at the TQ1/Conjugated Polymer P(NDI3N-T-Br) Interface

P1.001 ATR-FTIR spectroscopy and chemometric analyses of bumble bee secretions from hungry queens and workers

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Insects are widely known to manipulate plants in their environments in many ways. Scientists have recently discovered that pollen-starved bumble bees deliberately damage plants, producing flowers significantly earlier than they would otherwise [1,2]. This response reveals a wholly new dimension in the science of plant-pollinator interactions. It indicates some bees are not merely passive players in whether the timing of flowering matches their annual activity patterns. We hypothesise that pollen-starved bees produce secretions such as saliva, which are transferred into the leaf tissue, leading to an early flowering response. As-yet-unknown bioactive(s) in bumble bee saliva trigger this early flowering response.

Bombus terrestris (Hymenoptera: Apidae) queens and workers species (present in New Zealand) were used for chemical compositional analysis to test this hypothesis. Salivary glands, proboscis, and tarsi from 40 individual hungry bumble bees (queen vs worker) were collected. The possible isolates in bumble bee secretions were characterised using ATR-FTIR spectroscopy and chemometrics. Preliminary experimental results from IR spectra of each sample confirmed that protein is one of the possible components of all bumble bee secretions. Amide I (~ 1650 cm−1) and Amide II (~ 1550 cm−1) bands were observed, which are attributed to polypeptide/protein structure. We used chemometric analysis to identify and quantify the difference between starved queen and worker bumble bee secretions. Despite the similar chemical composition between secretions from salivary glands, proboscises, and tarsi, chemometric analyses showed significant differences between hungry queen and worker bumble bee salivary glands.

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P1.002 N-sulfonyl-4-(phenanthren-9-yl)-1,2,3-triazole functionalized silica as sorbent for the stir bar supported micro-solid-phase extraction of nitrosamines in water samples

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N-nitrosamines are class of emerging disinfection by-products that are widely found in several drinking water sources and they are formed during chlorination and chloramination of water. In this work, N-sulfonyl-4-(phenanthren-9-yl)-1,2,3-triazole functionalized silica sorbent was employed as effective sorbent for the extraction of four selected nitrosamines. The N-sulfonyl-4-(phenanthren-9-yl)-1,2,3-triazole functionalized silica sorbent was synthesized via two steps: first, the azide functionalization of silica and second, its click reaction with 9-ethynyl phenanthrene. The formed sorbent with high electron density and aromaticity was characterized using Fourier transform infrared spectroscopy, scanning electron microscopy, and an elemental analyzer. The sorbent was used in a stir bar-supported micro-solid-phase extraction (SB-μ-SPE) of the seven selected nitrosamines in 10 mL water samples, and in combination with gas chromatography-mass spectrometry (GC-MS). Extraction optimization was achieved with a sorbent mass of 25 mg, dichloromethane desorption solvent, 20 min extraction time, 10 min desorption time, and ionic strength of 1.0 g NaCl. Nitrosamines analytes calibration gave desired linearity range with R2 value of up to 0.9979 and a detection limit of between 0.21 to 0.25 ng mL-1. Relative standard deviation (RSD) and relative recovery experiments were tested using nitrosamines spiked at 1, 250, and 750 ng mL−1. RSD values were calculated in the range of 2.3–7.5% and the relative recoveries in the wastewater matrix successfully presented a range of 88.5–99.2%.

P1.003 Microfluidic Chip Fabrication: Micromilling to Application

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Microfluidics are an important technology for the biomedical industry and often utilised in our daily lives [1]. To facilitate the development of this technology, micromilling is proposed as an alternative method to conventional photo-lithography for fabricating microfluidic chips [2]. There remains uncertainty around what the ideal milling practices are and it is therefore important to investigate the milling process as well as the optimal parameters [3][4][5][6]. It is determined that the highest quality surface for 100 µm tools can be obtained at 60,000 RPM spindle speed with a 200 mm/min feed rate for PMMA, a common microfluidic material. Robust data was used to verify this relationship. Additionally, the process of fabricating microchannels with more complex geometries is investigated and full immersion wet milling solution is proposed to enhance surface consistency [6]. Milling tools 50 µm and smaller are experimented with to enhance the surface quality of microchannels and to allow for smaller fabrication. A functional Y-channel microfluidic chip is developed, allowing for the sorting of microparticles and/or microbes.

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P1.004 Suppression of Phosphine-Protected Au_9 Clusters Agglomeration on $SrTiO_3$ Particles Using a Chromium Hydroxide Layer

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Gold clusters have been shown to have great potential for use as co-catalysts in photocatalytic water splitting. Agglomeration of Au clusters deposited onto semiconductor surfaces into larger particles is a major challenge. Metal oxide overlayers can be used to improve the stability of Au clusters on surfaces and avoid their agglomeration. The aim of this work is to investigate the inhibition of phosphine-protected Au_9 clusters beneath a $Cr(OH)_3$ overlayer to agglomerate under conditions of photocatalytic water splitting (i.e. UV irradiation). Au_9 was deposited on the surface of $SrTiO_3$ using a solution impregnation method followed by photodeposition of a $Cr(OH)_3$ layer. After UV light irradiation for 7 hours for photocatalytic water splitting, uncovered Au clusters on $SrTiO_3$ agglomerated into larger particles. However, agglomeration was inhibited when a thin $Cr(OH)_3$ layer was deposited onto the $SrTiO_3$-Au_9 system. From careful XPS measurements, the chemical state of the overlayer is initially determined to be $Cr(OH)_3$ but upon heating at 200 ℃ for 10 mins it converts to Cr_2O_3. Through photocatalysis experiments it was found that the $Cr(OH)_3$ overlayer blocks the sites for O evolution reaction on the $SrTiO_3$-Au_9.

P1.005 Silver-loaded silica/HZSM5 nanocomposite as a novel SERS substrate for sulfur compound sensing in diesel samples

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Sulfur-containing chemical detection in petroleum products is regarded as a crucial area for research in both academia and industry. However, the utilization of surface-enhanced Raman scattering (SERS) spectroscopic techniques in that direction has not been well explored. This is mainly due to the complexity of the constituents in oil samples and to the intensive fluorescence emission produced by petroleum components. Herein, a novel combination of nanocomposites of silver-loaded silica and H-ZSM-5 (Si/Al2 = 150) material was developed and examined to identify different concentrations of dibenzothiophene (DBT) in commercial diesel fuel. Zeolitic materials assisted in lowering the fluorescence background, allowing for the approach of a low detection limit, whilst silver nanoparticles improved Raman signals related to DBT molecules. By interpreting the SERS peak at 1611 cm-1, which is connected to the aromatic CC stretching vibration, the DBT in diesel samples could be reliably detected up to 10-7 M of concentration. Surface and spectroscopic properties of the nanocomposite substrate before and after the combination of its components were compared using a variety of characterization techniques. Additionally, vibrational assignments of the main modes in the SERS spectrum of DBT were proposed based on literature and density functional theory (DFT) calculations. This work shall open a new direction in oil characterizations to apply the SERS method, being a non-destructive, fast and reliable alternative to conventional techniques.

P1.007 Synthesis and Reactivity of Organolanthanide(II) Hydrides

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Since the first report on the synthesis of a organolanthanide(III) hydride over 40 years ago, the field has witnessed enormous growth with hundreds of examples of organolanthanide(III) hydride based on every element in the lanthanide series. These complexes have now found applications in a range of industrially and academically important catalytic transformations, such as hydroboration, hydroamination and olefin polymerisation. In contrast, the synthesis and reactivity of lanthanide(II) hydrides is underdeveloped. Whilst there are three common lanthanides elements that are stable in the +2 oxidation state – Europium, Ytterbium and Samarium. There are only 7 examples of organolanthanide(II) hydrides, all based on Ytterbium.

The reactivity of these organoytterbium(II) hydrides is already beginning to diverge from that reported for the well-established organolanthanide(III) hydrides. For example, we have recently demonstrated that a low-coordinate organoytterbium(II) hydride could facilitate the first example of catalytic nucleophilic alkylation of benzene. This presentation will cover the new reactivity we have uncovered on our journey to extend the range of organolanthanide(II) hydrides beyond ytterbium to europium and samarium.

P1.009 Automation of Protein Crystal Harvesting

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Protein crystallography was first discovered in the mid-19th century, and X-ray crystal diffraction first used in 1912 [1]. The first true X-ray protein analysis was conducted on pepsin by Bernal & Hodgkin in 1934 [2]. Since then, protein X-ray crystallography has revolutionised science, assisting in genomics research, pharmaceutical development, and materials science [3]. Information about protein crystal atomic structures and their absolute configurations (chirality) has led to great advances in developing vaccines, categorising the human genome, and manufacturing exotic materials like metal-organic framework polymers [4–6]. However, preparation of protein crystals for X-Ray analysis is manual and needs to be automated for consistency and efficiency. We present a novel micro-manipulation system combining optimised borosilicate end-effectors with real-time closed-loop image processing. This system is capable of manipulating micro-objects in the <30 µm range, including irregularly shaped protein crystals. A motorised micro-manipulator is combined with an image processing algorithm to successfully grasp and transport micro-objects to a target location. This approach uses vector masking and closed-loop coordinate feedback to inform end-effectors of current and target locations, and separate them from micro-objects by contour area. The prosed approach resulted in an overall process improvement in automated pick-and-place operations with 25 µm micro-beads and irregularly shaped micro protein crystals. With the proposed system and recommended further work, the true capabilities of X-ray protein crystallography will be realised by automating the pick-and-place process.

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P1.010 Interpenetrating and patternable conducting polymer hydrogel coatings for neuronal recording and electrically stimulated drug delivery

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Neurological disorders are a significant global health issue affecting almost 6% of the population and often involve abnormal neuronal action potential firing and chemical signalling in the brain (1). Conventional systemic treatment options have limited ability to cross the blood brain barrier and have unwanted off-target effects. Alternative treatment options such as deep brain stimulation have enabled the treatment of various neurological conditions such as Parkinson's, epilepsy, and deafness (2). When targeting neurological disorders, devices that can deliver drugs while recording neural activity are desirable. Conducting polymer hydrogels (CPH) have emerged as a new class of biomaterials to functionalise electrode surfaces at the neural interface and for drug delivery (1-3).

This study presents the fabrication of CPHs, comprising the hydrogel gelatin methacrylate (GelMA), with the conducting polymers (CP) polypyrrole (PPy), or poly(2,4-ethylenedioxythiphene) (PEDOT), for drug delivery, and neural interface applications, respectively. Both CPH coatings form an interpenetrating network, confirmed by scanning electron microscopy and infrared spectroscopy, and can be covalently bonded to gold and photolithographically patterned. The CPH coatings were biocompatible, reversibly electroactive and electrochemically stable. The CPH comprising GelMA/PPy was loaded with glutamate, an excitatory neurotransmitter, and demonstrated electrically modulated release while delivering almost 14 times higher amounts of drug compared to conventional CP films. The CPH comprising GelMA/PEDOT was fabricated on microelectrode arrays, and successfully applied to record neuronal activity from primary hippocampal neurons. The CPH coatings presented here can form the components of a closed loop drug delivery system with the ability to release drug in response to cellular signalling.

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P1.011 Biological Applications of Gold Nanoparticles: From Cytotoxicity and Immunomodulation to Protein Crosslinking

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Gold nanoparticles are among the most versatile and adaptable nanomaterials due to their unique physical, chemical, and optical properties. Gold nanoparticles of different shapes and sizes, made from different sources, both with and without additional functionalization, have been used in various medical and biological applications including, but not limited to, imaging, signal enhancement, singlet oxygen generation, and as anticancer agents. In this presentation, three applications are highlighted. First, gold nanoparticles were synthesized using lemongrass extract in the presence or absence of different halide ions, to determine whether the cytotoxic and anti-proliferative effects of gold nanoparticles were altered. Second, gold nanoparticles were synthesized using different types of honey and the anti-inflammatory properties of these nanoparticles were investigated. These nanoparticles were found to inhibit lipopolysaccharide (LPS) induced interleukin-6 (IL6) production. Third, singlet oxygen, a form of reactive oxygen species (ROS), was generated from citrate-stabilized gold nanoparticles following irradiation by 532 nm laser pulses. The singlet oxygen targets aromatic amino acid residues in proteins and this mechanism has been used to create micron-scale protein crosslinks which can serve as a prototype for tissue engineering applications. Optimal cation concentrations for singlet oxygen generation and effect of ROS quenchers (sodium azide, mannitol) were also determined. Collectively, these results suggest that gold nanoparticles can be used for biological and biophysical applications such as cancer treatment, immunomodulation, and protein cross-linking.

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P1.012 The effect of pinholes on Josephson transport in aluminium-oxide tunnel junctions

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Josephson junctions are key components of quantum computers based on superconducting qubits. Although superconducting qubits are one of the most promising candidates to realise large-scale quantum computing, the materials science of Josephson junctions still limits their performance. Imperfections in Josephson junctions fabricated today are a source of energy dissipation and decoherence, as well as parameter drift and uncertainty. A possible explanation for this energy dissipation is the presence of microscopic metallic links called "pinholes" that might exist within the oxide tunnel barrier in the device.

Employing molecular dynamics and a tight-binding description of the system, we develop an atomistic model of Al/AlOx/Al Josephson junctions [1] as a method to resolve pinholes in the oxide tunnel barrier. Pairing this with a non-equilibrium Green's function (NEGF) approach we study quasiparticule transport through the device [2] to understand how pinholes may affect current. We additionally use a Bogoliubov de-Gennes (BdG) description of the system to study transport properties of the device in its superconducting state to understand how defects in the junction may affect the current-phase relationship in the device [3].

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P1.013 Reactive compatibilization of PP-PA6 blends using in-situ plasma treatment

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Blending different polymers is a well-known method to tailor material properties for specific applications requiring a unique set of characteristics [1]. However, most polymers are immiscible and require the addition of a compatibilizer to promote better adhesion between phases [2]. From an industry perspective, this method implies the use of chemistry techniques to manufacture the compatibilizer, commonly a graft copolymer miscible with both components [3], adding additional cost and complexity. In this work, we further study a proposed novel method for compatibilization of a PP-PA6 blend by applying an in-situ plasma treatment [4], comparing it with the standard use of PP-g-MAH as a compatibilizer for this blend [5].

Plasma is widely used as a surface modification technique, known to introduce polar oxygen groups such as C−O, C=O and O−C=O to the polymer [6-8]. It has the advantage of being a physical process and not requiring any reagents or solvents, thus more environmentally friendly. An air atmospheric pressure plasma jet (APPJ) was applied during compounding, introducing the same groups into the bulk structure of the polymers to promote the formation of hydrogen bonds between phases [9]. Pure PP was also melt-treated in an internal mixer to evaluate the introduction of functional groups. ATR-FTIR analysis showed the presence of C−O, C=O, and -OH bands, indicating the formation of carboxyl or ester groups. The plasma-treated blends presented a slight increase in mechanical properties over the untreated blends, explained by a finer phase dispersion observed through SEM images.

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P1.014 Non-linear pressure effects on Tc and Jc in Phosphorous doped BaFe2As2

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Iron-based superconductors (FeSC's) fit unambiguously under the umbrella of 'unconventional superconductivity', with many representative samples displaying non-Fermi liquid normal-state properties and quantum critical behaviours. The fact that they often have a huge range of doping possibilities, resulting in a broad range of superconducting and normal-state properties, means they provide a fascinating playground for exploring which material parameters have measurable links to the strength of superconductivity.

In the study of P-doped BaFe2As2, one of the most promising FeSC materials, application of pressure is one such parameter. However, previous reports of pressure dependence on this material have produced seemingly incongruent results. Very small pressures (< 10 MPa) have been shown to decrease values of the superconducting critical temperature (Tc) [1], whereas large pressures (1 < 10 GPa) clearly result in increased values of Tc [2].

We present an investigation into the effects of externally applied hydrostatic pressures on the superconducting properties of P-doped Ba122, with the aim of coalescing all these observations into a single coherent interpretation. Our measurements unveil a distinct non-linear dependence of Tc on pressure, with critical current values following suit. This behaviour is characterised by a steep initial decrease for pressures up to 0.4 GPa, with values diminished by as much as 50 %, followed by a recovery of the 0 GPa values near 0.8 GPa. This non-linear behaviour, which smoothly interpolates other groups data from high and low pressure regimes, is interpreted as being a direct result of anisotropic strains induced in the material.

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P1.015 Enhanced ganciclovir activity against cytomegalovirus in combination with nanocarrier delivered quercetin

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Congenital cytomegalovirus (CMV) infection affects 30,000 – 40,000 infants in the United States each year, frequently leading to progressive hearing loss, with potential severe neurological damage and mortality [1]. CMV infection requires long-term administration of nucleoside analog antivirals such as ganciclovir (GCV), a therapy frequently limited by GCV-induced toxicity. The aim of this research was to investigate combination therapy of GCV and two bioactive excipients, poloxamer 188 (P188) and quercetin to reduce GCV dosage. Quercetin is a natural flavonoid exhibiting antiviral activity against CMV by a mechanism distinct from GCV, but is poorly soluble, limiting its use as a therapeutic [2]. To overcome this challenge, quercetin was co-formulated with P188 and assessed in-vitro [3]. Quercetin-P188 (QP188) formulations yielded modest CMV inhibition, with a selectivity index of 11.4, contrasted with a GCV selectivity index of 95 in fibroblast cell culture. More significantly, when co-administered with GCV, QP188 exhibited an additive interaction at low concentration (2.6 µM quercetin / 0.1 mM P188) and synergistic interaction at high concentration (26 µM quercetin / 1 mM P188). Blank P188 also interacted synergistically with GCV, supporting a role as a bioactive excipient. Fluorescence microscopy revealed QP188 on the cell membrane and accumulation in mitochondria, suggesting P188 may modulate mitochondrial processes relevant to CMV infection [4]. Intraperitoneal injections of sub-therapeutic doses of GCV and QP188 in a mouse CMV model protected the mice from CMV-induced hearing loss, validating that the combinatorial therapy provides otoprotective as well as antiviral activity [5].

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P1.016 Controlling spins with THz pulses

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Strong photon pumping can drive matter to unique transient states and drastically change its magnetic properties. This may lead to development of new nanoelectronic devices. Particularly high field intensities can be achieved for irradiation at THz frequencies. The THz field directly causes coherent precession of spins via the Zeeman interaction. In metals, an important role is also played by THz field-induced direct excitations of conduction electrons to higher energies. This leads to incoherent quenching of magnetism on a femtosecond time scale, which competes with the coherent Zeeman torque [1].

THz photons can also coherently excite soft polar phonons into nonlinear regime enabling new couplings to the spin system. This is particularly important in insulators and may lead to a change of magnetic order. Phonons excited in a controlled way may break the symmetry between two antiferromagnetically coupled moments to form a ferrimagnet [2] or modify magnetic interactions so that the system turns from a collinear antiferromagnet to a canted weak ferromagnet [3].

We employ first principles calculation methods to reveal optical and magneto-optical properties properties of the strongly nonequilibrium THz pumped state. These are used to understand interesting experimental results associated to THz induced toggle switching in the intensively studied GdFeCo metallic systems. We also investigate microscopic aspects of nonlinear spin-phonon interactions leading to magnetic order modifications. We have evaluated magnetic exchange interactions under influence of specific non-equilibrium phonon populations for prospective systems. Probable phonon mode populations are obtained using our method developed for describing phonon distribution dynamics [4].

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P1.017 Conducting oligomers grafted biopolymer for transient electronics

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Transient electronics is an emerging field where electronic devices or circuity are intentionally designed to a loss of function irreversibly. However, current methods involve the use of inorganic materials that are potentially toxic or require high energy processing. In this project we aim to synthesise novel organic conductors that degrade under physiological conditions into environmentally benign by-products for use as transient circuitry.

In this project, we developed a novel approach to transient organic electronic materials, based on conjugated oligomers grafted onto the biodegradable polymer, polycaprolactone (PCL). This approach allowed encourage the oligomers to form π-π stacked configuration and crystallised domains that provide the electroactivity, whereas the PCL component provide the degradation, enabling the synthesised construct to be broken down into non-toxic, low-molecular weight components. Different lengths of oligomers of 3-hexylthiophene (3HT) were synthesised and then functionalised with azide groups to provide a handle for attachment. PCL, with different density of alkyne modification were also synthesised and was then grafted on the O3HT oligomers. The physical and electronic of the polymers are studied using techniques such as XRD, AFM, SEM, cyclic voltammetry.

P1.019 Solar Cell Fabrication Lab Teaching during the COVID-19 pandemic

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The Solar cell Lab, established by Professor Maan Alkaisi, is an essential element of the Nano Engineered Device course at Electrical and Computer Engineering, University of Canterbury, introducing and demonstrating solar cell fabrication processes to 400-level students. [1]

The lab has attracted students from multiple departments and the number of enrolled students increased from less than 20 in 2011 to over 60 in 2022. Some students continued their research in nanotechnology after this course. Students are expected to fabricate a fully functional solar cell from a plain, silicon wafer that they received at the beginning of the lab session. They are expected to have hands-on experiences in semiconductor fabrication processes such as impurity diffusion, photolithography, thin film depositions, and etchings, as well as device characterizations such as solar simulated dark and light IV characteristics, thin film thickness, and surface morphology characteristics. The highest PCE of these students-made solar cells is nearly 10 %.

Since the COVID-19 pandemic, several measures were implemented to minimize virus transmissions, including the maximum number of students for each session. Therefore, the original lab session arrangements are modified. Videos were taken during wafer preparations and lab sessions to ensure the lab is available for all students who enrolled in the course.

With the change in lab session arrangements, better interaction with students can be observed during lab sessions. TAs can have breaks between streams, and more preparation times between sessions. Despite the challenges, students are still able to achieve similar cell performance compared to pre-COVID years.

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P1.020 Sustainable powders for laser-assisted additive manufacturing

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Sustainable materials are being used more commonly with additive manufacturing (AM) technique to enable the manufacture of functional products in a sustainable and economically efficient way [1]. Selective laser sintering (SLS), is an AM technique that shows potential in fusing and solidifying biomass powders into 3D porous materials, paving the way in technical applications [2, 3]. However, because of the low thermal stability of biomass under laser sintering, petroleum thermoplastic polymers, such as nylon, are often mixed with biomass powders to increase their processability for SLS applications [4]. In this latter situation, the interfacial interactions between biomass powder and thermoplastic remain one of the most important challenges that need to be addressed [5]. It is therefore important to develop a method that enables SLS printing of biomass powders directly.

In this work, we have developed an AM process for biomass powders using a laser sintering process with a commercial CO2 laser. The laser system is equipped with a chamber that has nitrogen flowing through it to prevent combustion of the powder. By using a layer-by-layer deposition technique, followed by laser sintering, a 3D structure can be directly printed from vegetal waxes and lignocellulosic composite powders. The morphological, chemical, and mechanical properties of the prepared 3D structures have been characterised by scanning electron microscopy (SEM), Fourier transform infrared spectrometer (FTIR) and dynamic mechanical thermal analysis (DMTA). The processability of wax powders with different particle sizes has been studied. This method is simple and requires no additional chemical or physical process, and it is potentially scalable for industrial applications.

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P1.021 Coherent Raman spectro-microscopy using multiple-plate continuum

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Coherent Raman scattering (CRS) has attracted increasing attention for the ability toward background-free molecular-specific acquisitions without exogenous labeling. Nevertheless, practically useful sensitivity and specificity largely rely on an advanced laser system with enough excitation power to offer sufficient signals and unconstrained wavelength tuning range to match the desired Raman modes. The current benchmark is the combination of a pico- or femtosecond mode-locked solid-state oscillator and a synchronously pumped optical parametric oscillator (OPO) [Science 2008, 322 (5909)]. Despite its great popularity and success, the phase-sensitive nature of degenerate OPO hampers its access to low-frequency Raman shifts, and has no freedom to independently adjust the second wavelength, preventing itself from electronic pre-resonance (EPR) detection for desirable molecules [J. Phys. Chem. Lett. 2018, 9 (15)].

Here, we demonstrated CRS spectro-microscopy driven by a multiple-plate continuum (MPC) supercontinuum laser source [Optica 2014, 1 (6), Opt. Express 2019, 27 (11), Front. Photon 2022, 3 (937622)], whose octave-spanning bandwidth (600-1300 nm) and high spectral energy density (~1 nJ/cm^-1) offer capabilities of dual-wavelength tunability, facilitating the spectroscopic characterization in the entire Raman active region (0~4000 cm^-1), EPR detection, and single-wavelength CRS imaging. As a proof-of-concept experiment, we interrogate Raman modes of pure acetonitrile solution across fingerprint, silent, and C-H stretch Raman regions. In addition, we presented the imaging modality of the MPC-CRS system via a Drosophila brain. Finally, highly sensitive EPR detection is exemplified with the C=C mode of a commercial Alexa 635 fluorescent dye. We envision that benefiting the wavelength tunability in MPC-CRS system, it is valuable in applications such as highly sensitive EPR mode imaging as well as multiplex CRS imaging [Opt. Express 2022, accepted].

P1.022 Alignment and insulation of Fe-Si nanocrystalline alloy for magnetic composite cores

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Nanocrystalline soft magnetic materials are fundamental to today's electronic and electrical engineering industry. In particular, there has been great interest in iron (Fe)-based alloys due to their excellent soft magnetic properties, high saturation magnetisation and permeability, low core loss, and near-zero magnetostriction. The family of soft magnetic materials based on amorphous Fe-Si-B-Nb-Cu alloys with a dispersion of Fe-Si nanocrystalline phase reinforced ferromagnetic composites have shown excellent magnetic properties in the high frequency range, and lower power losses compared to iron powder cores. However, the bulk resistivity value of this alloy is in the 10-4 Ω-cm range, which will inevitably contribute to higher eddy current losses.

Decreasing eddy current losses is usually achieved by increasing the sample's resistivity. Insulating coatings using organic and inorganic layers have already been demonstrated with the latter providing better thermal properties and mechanical strength.

In this study, we report a new procedure for electrically insulating the surface of anisotropic Vitroperm 800 flakes, an amorphous Fe-Si-B-Nb-Cu alloy by VAC Vacuumschmelze GmbH & Co., aimed for inductive power transfer applications. To preserve the excellent intrinsic magnetic properties of Vitroperm, we managed to achieve an alignment of the Vitroperm flakes through applying mechanical pressure. The electrical insulation of the alloy was achieved through organosilane coating followed by heat treatment to remove the organic moieties. We found that the organosilane coating and subsequent high-temperature treatment has little effect on the magnetic properties. More importantly, a huge increase in the resistivity of the surface-insulated Vitroperm, compared with the untreated Vitroperm, was observed.

P1.023 Evaluation of the hypericin-loaded nanostructured lipids potential as a strategy in vulvovaginal candidiasis therapy

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Vulvaginal candidiasis (VVC) currently represents a major health challenge due to its high incidence and relapses, which may be due to host-related factors, such as immune system compromise, or pathogen-related factors, such as resistance to antifungals.Therefore, it is necessary to study new treatment alternatives, as the use of substances of natural origin, such as hypericin (HYP), which has antifungal action. However, there are many challenges in its clinical use, due to its physicochemical characteristics like rapid hydrolysis in low pH alkalis and in the presence of light, in addition to pharmacokinetic characteristics, such as low oral absorption, extensive hepatic metabolism and rapid elimination. Therefore, its incorporation into nanostructured lipid carriers (NCL) for vaginal administration is an interesting option that enables its use. The objective of this work was to evaluate the potential of HYP-loaded NLC as a strategy in VVC therapy. NLC and HYP-loaded NLC were obtained by sonication at 35% amplitude for 5min, with the aqueous phase composed by poloxamer 407 and the oil phase composed by polyoxyethylene 40 stearate, capric/caprylic acid triglycerides and ethoxylated hydrogenated castor oil. NLC and NLC-HYP were characterized by dynamic light scattering technique to evaluate the average particle size distribution. The in vitro minimum inhibitory concentration of the NLC and HYP-loaded NLC against Candida albicans was also evaluated. The in vitro inhibition effect of the systems was tested to reduce the planktonic viability of C. albicans. NLC and NLC-HYP did not show instability characteristics, such as aggregation and phase separation, and the mean hydrodynamic diameter, polydispersity index and zeta potential values were 133.7 and 125.9 nm, 0.19 and 0.22, and -20.8 and -30.3 mV, respectively, on day 7. NLC showed no activity against C. albicans, but the NLC-HYP had a potential antifungal activity against the analyzed strain. In addition, in the in vitro inhibition assay, NLC-HYP treatment showed a significant log10 reduction in the planktonic viability of C. albicans in relation to the negative control (yeast nitrogen base). The results suggest the antifungal potential of the system as an effective strategy in VVC therapy.

P1.025 Pilot-scale production of expansile nanoparticles: Practical methods for clinical scale-up

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A significant challenge in translating nanoparticle technologies to the clinic is the requirement to produce materials on a large-scale. Scaling nanoparticle production methods is often non-trivial, and the success of these endeavors is frequently governed by whether or not an intermediate level of production (termed "pilot-scale" production) is achievable. Pilot-scale production at the one-liter scale serves as a proof-of-concept that large-scale production will be possible. Here, we describe the pilot-scale production of the expansile nanoparticle (eNP) technology including verification of activity and efficacy following scaleup. We describe the challenges of sonication-based emulsification procedures and how these were overcome by use of a Microfluidizer technology. We also describe the problem-solving process that led to pre-polymerization of the nanoparticle polymer—a fundamental change from the lab-scale and previously published methods. Furthermore, we demonstrate good control over particle diameter, polydispersity and drug loading and the ability to sterilize the particles via filtration using this method. To facilitate long-term storage of these larger quantities of particles, we investigated six lyoprotectants and determined that sucrose is the most compatible with the current system. Lastly, we demonstrate that these changes to the manufacturing method do not adversely affect the swelling functionality of the particles, their highly specific localization to tumors, their non-toxicity in vivo or their efficacy in treating established intraperitoneal mesothelioma xenografts.

P1.027 Direct conversion of CO2 to solid carbon by Ga-based liquid metals

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The direct conversion of CO2 to solid carbon could offer a pathway towards mitigating anthropogenic CO2 emissions and may lead to a negative emissions technology if implemented at scale.[1] Unfortunately, the solid nature of the product results in deactivation due to coke formation being a significant challenge.[2] In this work, we demonstrate that gallium based liquid metals can effectively activate the CO2 molecule, resulting in the formation of solid carbonaceous products.[3] Due to the liquid nature of the metal, deactivation is effectively mitigated, resulting in an overall robust process. Furthermore, a straightforward metal regeneration process has been demonstrated, enabling a scalable Ga | Ga3+ chemical looping process that is capable of effectively converting CO2 into solid carbon and O2 at temperatures as low as 200 C.

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P1.028 Multicomponent Metal-Organic Frameworks (MOFs) Using Amino Acid and Peptide Ligands

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Metal-organic frameworks (MOFs) are porous materials that built of metal ions or clusters and organic ligands.1 The organic ligands act like bridges to link the nodes and form open networks. The pores in these MOFs make them useful for applications like sensing, catalysis, and storage since guest molecules can be captured in the pores. The ligands used to build up the MOFs are usually rigid, but there has been an interest in flexible ligands, such as amino acids and peptides.2-5 All studies to date have used one kind of ligand. In this project, we will focus on using combinations of amino acids (or peptides) as ligands. The MOF structures may resemble proteins and therefore deliver unique catalytic properties. Other properties, like chirality, biocompatibility, and low cost may make them useful in applications like drug delivery and sensing.

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P1.029 Chitosan-Coated Selenium Nanoparticles Suppress Metastasis and Enhances Chemosensitivity of Glioma Cells

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Selenium nanoparticle (SeNP) has been developed to overcome the limitations of using selenium which are narrow safe range of exposure, low water solubility and dispersity. SeNP is a novel selenium species with potent anticancer activity and low toxicity. In this study, chitosan-coated SeNP (Cs-SeNP) was developed to further stabilize SeNP and to test its effects against glioma cell line, U87 cells. The effect of the formulated nanoparticles on cell growth of U87 cells, both monolayer and 3D-tumor spheroid cultures, was evaluated using MTT assay and spheroid volume determination, respectively. The results suggested that SeNP and Cs-SeNP reduced the cell viability in dose-dependent manners. Cs-SeNP provided a stronger effect of 3D-tumor spheroid growth inhibition compared with SeNP. Effects of SeNP and Cs-SeNP on cell migration and cell invasion of U87 cells were determined using transwell assay. Cs-SeNP exhibited a greater effect of inhibiting cell migration and cell invasion than those of SeNP. The possibility of applying SeNP and Cs-SeNP to enhance the sensitivity of chemotherapeutic drug, 5-FU, against U87 cells was determined in 3D-tumor spheroid culture. An improvement of 5-FU sensitivity was observed in Cs-SeNP treated cells. The study of cellular uptake of the nanoparticle in U87 cells indicated the higher uptake rate of coumarin-6 labeled Cs-SeNP than SeNP. The capability to pass through blood-brain barrier (BBB) of Cs-SeNP was confirmed in in vitro BBB model. Taken together, Cs-SeNP provided the exceptionally performance which could be an alternative therapeutic strategy for the future glioma treatment.

Keywords: Selenium nanoparticle; Chitosan; Glioma; Metastasis; Drug sensitivity; Blood-brain barrier

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P1.030 Using geometrical modelling to determine key mechanical variables of the fibre-fibre interactions in calamus manau rattan.

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There is a call to address the issues of climate change, known to be exacerbated through the unhindered use of fossil fuels, and a throwaway society. There are environmentalists that continue to see the beauty and strength in the natural world and continue a preference of these things. There are also the traditionalists who continue the use of natural materials because they can. Examples of which are seen in the sporting codes of cricket and equestrian polo. The cricket bat which must according to international rules must be made from the timber willow [1]. The mallet used in polo, not expressed in the international rules [2], is given a preference by the leading teams of players to be made from a Rattan cane.
Following an investigation into the performance of the shaft of the polo mallet we consider the use of a geometrical model to represent the shaft on a micro-scale [3]. At this scale we introduce the individual fibres and assume a symmetrical order for the entire cross-section. This assumption then allowed us to determine the second moment of area which is a key variable in calculating shaft response to, both static and dynamic, mechanical loading [4].
This poster shows the modelled ratan shaft and the associated mathematical model produced.

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P1.031 Active Machine Learning for Efficient Predictions of the Functional Properties of Millions of Novel Layered Van der Waals Heterostructures

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There are currently more than 6000 theoretically predicted 2-dimensional (2D) van der Waals materials with functional and structural properties that can be significantly different from their 3-dimensional counterparts. The combination of more than one monolayer to form heterostructures can potentially give rise to an extremely large set of structures with unique and exotic properties that will drive novel industrial applications. However, even combining only two different monolayers into bilayers, the number of possible heterostructures exceeds millions, making the analysis of the properties of this class of materials impractical from both an experimental perspective and using conventional ab-initio computational models. Here, a time and resource-efficient active machine learning approach has been used to create a database containing the functional and structural properties of millions of van der Waals layered structures. We predicted the interlayer energy, elastic constant, bandgap and piezoelectric constant of layered materials composed of two different 2D structures mainly in view of their application in energy conversion devices (e.g. photocatalysis). Our active machine learning models can predict results of computationally expansive approaches (i.e., density functional theory) with high accuracy.1,2,3

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P1.032 Diffusion and exchange in nanoporous materials studied with Magic Angle Spinning (MAS) NMR diffusometry

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Nanoporous materials such as zeolites are widely used in chemical catalysis, separation and storage at laboratory and industrial scale. More recently, Metal Organic Frameworks (MOF's) have attracted attention due to their nearly unlimited configurability and adaptability. This, in turn, calls for rigorous and comprehensive characterization of newly developed MOF's.

Here we report on the dynamics and mobility of hydrocarbons in the MOF NU-1000 [1] by means of nuclear magnetic resonance (NMR). One key element is the use of magic angle spinning (MAS) [2]. This reduces NMR relaxation of strongly adsorbed guest molecules in the porous host framework, thus enabling to resolve spectral features of the adsorbate on the chemical shift scale. Furthermore, one and two dimensional NMR diffusometry [3,4] can be used under such condition which yields adsorbate mobility, molecular exchange and preferential distribution within the MOF network. In particular, we studied how the mobility of benzene responds to different adsorbate loadings. Furthermore, we demonstrate that benzene at higher loadings partitions in a bulk phase which is in fast exchange with a layer adsorbed along the pore walls. We will also report on mixture diffusion of benzene and hexane in the same MOF.

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P1.033 Computational modelling of heterogeneous catalysis: The challenges posed by electro- and nano- catalysts

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Heterogeneous catalysis encompasses a class of catalytic reactions in which the phase of the catalyst is different to that of the reactants. Typically the catalyst is a solid while the reactants are either liquids or gases. Heterogeneous catalysis plays a vital role in a number of existing processes, such as fertilizer production, fuel cells and catalytic converters in automobiles. Two aspects of heterogeneous catalysis of interest to my research group are electrocatalytic reactions and reactions using nanoparticle catalysts. However, both of these present significant challenges for computational modelling.

In this poster I will present research ongoing in our group in both electro- and nano-catalysis.
I will present results concerning electrocatalytic modelling where (i) we explicitly consider the effect of the solvent environment and the applied potential1 and (ii) the presence of protons is found to profound affect reaction selectivity.2 I will also present results on the structural sensitivity of nanoparticle catalysts3,4,5 and methods under development in our group to efficiently predict nanoparticle morphology.6,7

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P1.034 Magnetic properties and spontaneous anomalous Hall effect in bulk hexagonal MnTe - an unconventional antiferromagnet

MSc. Kacper Kluczyk[1], Dr. Katarzyna Gas[2], Dr. Michał Grzybowski[1], Dr. Michał A. Borysiewicz[3], Dr. Tomasz Fas[1], Dr. Jan Suffczynski[1], Dr. Pawel Skupinski[2], Prof. Krzysztof Grasza[2], Prof. Andrzej Mycielski[2], Prof. Maciej Sawicki[2], Dr. Marta Gryglas-Borysiewicz[1]

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A recently identified third robust magnetic phase, dubbed altermagnetism, is characterized by a compensated magnetic order (as in antiferromagnets) with opposite-spin sublattices connected by crystal-rotation symmetries, and by band structures with broken time-reversal-symmetry and alternating sign of the spin splitting in the momentum space [1]. Semiconducting hexagonal MnTe with energy gap of ~1.3 eV belongs to this class offering unprecedented spintronics functionalities. It is therefore timely and important to expand the envelope of material growth methods, particularly to investigate its properties in greater detail.

Here we report on magnetic and electrical properties of bulk hexagonal MnTe. The material is grown from the vapour phase via reaction of tellurium vapors with manganese powder at a temperature aiming to reduce the formation of unwanted phases, like MnTe2.

All magnetic and electrical transport results point to antiferromagnetic phase transition at ~310 K, in agreement with the previous studies [2,3] but a weak signatures of antiferromagnetic MnTe2 with its Neel temperature close to 90 K is still detected. A significant rise of resistivity is observed below 20 K, indicating activated character of the charge transport. Magnetization studies reveal the presence of a sizable magnetic anisotropy with a magnitude expected to hexagonal antiferromagnets [3]. Most importantly, a clear spontaneous anomalous Hall effect, an effect specific to ferromagnets, is detected at temperatures as high as 240 K confirming the breaking of the time-reversal-symmetry in this antiferromagnet, and so making hexagonal MnTe a worthwhile spintronics material.

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P1.035 Electron correlation effects in spin-polarized quasi-one-dimensional quantum fluid

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In this work, we have studied the electron correlation and confinement effects of spin-polarized quasi-one-dimensional (1D) electron fluid at various densities using quantum Monte Carlo (QMC) method. The ground-state properties including structure factor, pair correlation function, momentum density, and correlation energy are calculated for several values of spin-polarization ζ=|N_↑-N_↓ |/N, where N_(↑(↓)) denotes number of up(down) electrons at various values of density parameter r_s. The Tomonaga-Luttinger exponent is found by fitting the QMC momentum density data with an appropriate fit function around k~k_F. The TL parameters give the detailed description of low energy physics of spin-polarized electron fluid. Further, we have explored the finite width confinement effect of correlation energy in quasi-1D spin-polarized electron fluid.

P1.036 Adaptive cellular designs for the monitoring of the structural integrity of conductive materials using additive manufacturing route

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Additive manufacturing is a quite recent route for processing materials, which offers a large degree of freedom in designing structures with shape complexity and multi-functional performance. In this study, fused deposition filament is considered to manufacture a new generation of materials capable of diagnosing their structural integrity by capturing the deformation that is correlated to electrical resistivity variation. The idea is to design open circuits within the material, which when subjected to mechanical loading, electric circuits are closed, allowing to capture the loading response in terms of electrical conductivity variation. The proof of concept is performed based on airy cellular structures containing both nonconductive PolyLactic Acid (PLA) material combined with conductive Acrylonitrile Butadiene Styrene (e-ABS). Simulation of the coupled mechanical – electric problem is performed using Comsol multi-physics. The fabrication of open circuits within the cellular materials is undertaken according to the predictive analysis. The characterisation of the electric response of the cellular material is performed under compression loading using an open source Arduino measurement circuit. The results show that the predictive analysis shows a drastic increase in the voltage followed by a steady-state regime when loading is increased. The experimental monitoring demonstrates the same sudden increase in voltage but with an irregular asymptotic trend. This study concludes that the amount of loading needed to compromise the integrity of a structure can be captured using the developed approach. The monitoring of lower deformation levels requires a more complex design that will be addressed in a future development.

P1.037 Three anti-wrinkle European Renaissance recipes as sustainable cosmetic alternatives

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Cosmetics have provided an arena for chemical experimentation for millennia. And while there is burgeoning interest for historians about the historical cosmetics, there is a surprising dearth of scientific, lab-based analysis especially regarding natural based ingredients. The chemical composition of three European Renaissance blemish and wrinkle-removing recipes were analysed to understand the effectiveness of their intended purpose and any dermatological benefits. The first was rosemary in white wine, the second, a combination of myrrh and hard-boiled egg whites and the third a paste made from deer antler, bean flour, and rosewater. Infrared spectroscopy was used for insight into the chemical makeup and relative amounts of the components in the final products. After which liquid chromatography with mass spectrometry (LC-MS) was used for protein analysis and gas chromatography with MS (GC-MS) was used to identify the compounds within the formulations.

The FTIR spectra of the rosemary and white wine revealed primarily esters and acids, while those of the myrrh and egg white extract showed mostly proteins, esters, and acids. FTIR of the paste made from deer antler velvet, bean flour and rosewater showed the presence of proteins, fatty acids, and starch. GC-MS and LC-MS analysis on the three recipes revealed the identity of numerous volatile compounds and proteins with medicinal and skincare applications used in the cosmetics industry. The results of this study provide insight into why these recipes were used and were so ubiquitous in the European Renaissance and possible further application as a sustainable alternative in the cosmetics industry.

P1.038 Exchange/Zeeman Competition in the Rare-Earth Nitrides and the Resulting Magnetic Compensation

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The rare-earth nitrides are the only known series of intrinsic ferromagnetic semiconductors, with a range of magnetic behaviours stemming from the contribution of both spin and orbital 4f moments. The similar chemistry of the rare-earths and the common structure of the nitrides simplifies their combination in superlattices and solid solutions. Recent studies of rare-earth nitride superlattices have shown enhanced superconductivity and magnetic exchange spring behaviour that results from the competition between the Zeeman and Exchange interactions. Yet, little has been published to date exploring the combination of these nitrides in solid-solutions.

We show (with reference to magnetometry, XMCD and anomalous Hall effect measurements) that the same Exchange/Zeeman competition that leads to a complex twisted magnetic phase in superlattices manifests quite differently in solid solutions. Leading, where an orbital-dominant ferromagnet (SmN) is paired with a spin-only ferromagnet (GdN), to a composition exhibiting a net zero magnetic moment (A compensation point).

P1.039 Direct laser patterning of semi-transparent organic solar cells with average visible transparency (AVT) approaching 50%.

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In recent years, the most important green energy source is solar cells, in order to match the application, semi-transparent solar cells have been developed, which can replace ordinary glass, let that become have converting light into electrical function glass, and apply power supply for electronic products such as building, car and watch. Therefore, the development and application of semi-transparent solar cells are an indispensable part of the human future. In this work, we demonstrate a direct laser patterning of organic solar cells (OSC), and the cell power conversion efficiency (PCE) and average visible transparency (AVT) can be controlled through pattern design. At an optimized laser pattern of hexagon width of 120 µm and spacing of each hexagon 30 µm, the process successfully maintained the power PCE by over 10% and AVT at 50%. The WO_3 covered after devices plays an important role in direct laser patterning because it can effectively suppress the detachment of the cathode and the short circuit with the anode caused by the thermal effect of the electrode during the laser process. Successful operation of the direct laser patterning of OSC is a simple and fast technology for processing semi-transparent solar cells.

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P1.040 Recent Advances in Molecular Multimetallic Systems: Design and Synthesis of Polyoxometalate-Based Novel Systems

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Polyoxometalate (POM) chemistry is an important branch of the molecular nanotechnology. Over the past decades, POMs as molecular metal–oxide clusters have attracted extensive interest because of their unmatched range of physical properties that make them ideal building blocks for the development of a wide variety of structures and advanced multifunctional materials. They have been applied in many research fields, such as optics, magnetism, biological medicine, energy storage and catalysis (1-3). Further, these molecular materials from low-cost, earth-abundant elements and with well-defined structures are a major focus since they provide an ideal platform for understanding the reaction mechanisms of various processes. However, the control and manipulation of molecules with predefined properties tailored to specific applications is a great challenge.
Herein, I present about our current work, which is focused on the synthesis and development of multifunctional systems based on POMs and to harness their properties for practical applications.

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P1.041 Hole-Mediated Photocatalysis in Hydrated Mixed-Phase o/h-WO3 Core-Shell Nanoribbons

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We have discussed two different kinds of self-decorated WO3 nanoribbon heterostructures in this study. Hydrothermal-calcination techniques are used to produce these heterostructures. The mixed-phase sample (h-WO3/o-WO3.H2O), which is hexagonal (h) and orthorhombic (o), develops an amorphous/crystalline core-shell structure. The monoclinic (m)-WO3 calcined sample produces a crystalline nanodot/nanoribbon morphology. These synthesized nanosystems are abundant in oxygen vacancies and show photoabsorption that extends into the near-infrared (NIR) spectrum. Electrochemical spectroscopy shows that the core-shell structure has a lower charge-transfer resistance than the dot/nanoribbon structure. The mixed-phase has a stronger photocatalytic methylene blue (MB) degradation than the dot/nanoribbon under visible and monochromatic light. The mixed-phase has a stronger photocatalytic methylene blue (MB) degradation than the dot/nanoribbon under visible and monochromatic light. The underlying process demonstrates that there are three reasons why the mixed-phase core-shell is better than other crystalline phases. (1) Effective carrier separation at the core-shell/mixed-phase junction, (2) Intercalated water from the medium/o-WO3.H2O phase, and (3) electron trapping sites. The photogenerated electrons are trapped by the oxygen defects, leaving open holes. Water molecules can easily diffuse and intercalate thanks to the mixed-tunnel phase's structure. In order to create hydroxyl radicals for activated photocatalysis, the intercalated water molecules easily interact with the mobile holes. All of these elements helps WO3 nanoribbons to function photocatalytically better.

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1. Hydrated Orthorhombic/Hexagonal Mixed-Phase WO3 Core−Shell Nanoribbons for Hole-Mediated Photocatalysis
Manju Kumari Jaiswal and Biswajit Choudhury*
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https://doi.org/10.1021/acsanm.1c04267

P1.043 Multifunctional ultrafine inorganic nanomaterial aerogel as high performance chemical sensor platform

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We report a facile production of a multifunctional porous inorganic nanomaterial aerogel by controllable surface chemistry of a functionalized SWNT (fSWNT) hydrogel platform for the first time. The versatile functional inorganic nanoparticles can be incorporated uniformly on the porous 3D fSWNT hydrogel platform through a facile dip coating method at ambient conditions. The morphology of the multifunctional inorganic aerogel is manipulated by designing the fSWNT hydrogel platform for different requirements of applications. In particular, Pt-SnO_2 aerogels exhibit high porosity and uniformly distributed ultrafine Pt and SnO_2 on the fSWNT platform with controllable particle size (1.5-3.5 nm), which result in significantly high surface area (393 m^2/ g). The ultrafine Pt-SnO_2 aerogels exhibit highly sensitive (14.77% at 5 ppm) and selective NO_2 sensing performance even at room temperature due to the increased active surface area and controllable porous structure of the ultrafine aerogel, which can provide fast transport and penetration of a target gas into the sensing layers. The newly designed multifunctional inorganic aerogel with ultrahigh surface area and high open porosity is a prospective materials platform of high performance gas sensors, which could be also broadly expanded to widespread applications including catalysis and energy storages.

P1.044 Enhanced piezoelectric modulus of wurtzite AlN by ion beam strain engineering

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Aluminium nitride (AlN) is a functional III-V semiconductor with high mechanical and thermal stability. Integration of AlN in optoelectronic and electronic components is simplified as it is compatible with complementary metal-oxide semiconductor (CMOS) technology. The piezoelectric modulus of wurtzite Aluminium Nitride (AlN) is a critical material parameter for acoustic wave resonators, ultimately contributing to the energy efficiency and achievable bandwidth of modern communication devices. Here, we report that the introduction of metallic point-defects (Ti, Zr, Hf) improves the piezoelectric modulus of as-received, unstrained, epitaxially grown AlN. The metals are incorporated by ion implantation with an acceleration energy of 30 keV to a fluence of 1015 at.cm-2, which causes an elongation along the wurtzite c-axis. The stored internal strain energy increases the piezoelectric polarization of the thin AlN layer, which can equivalently be described by an enhancement of the piezoelectric modulus d33. The incorporation of 0.1 at.-% Ti enhances the piezoelectric modulus by ~30 %; significantly exceeding gains by alloying with the same amount of Sc [1-3].

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P1.045 Electrochemical measurement of serotonin concentration in platelets using single particle collision on microelectrode

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Serotonin is one of the human neurotransmitters and plays a very important role. It is a well-known fact that abnormal serotonin levels are associated with various psychiatric disorders, such as depression, schizophrenia, and obsessive-compulsive disorder [1]. Therefore, it is very important to detect the concentration of serotonin sensitively. However, the level of serotonin in the blood is very low and not easily detectable. This is because most of the serotonin in the blood is stored in platelets. Therefore, a new method for detecting the concentration of serotonin in platelets is needed. This study is a method to confirm the concentration of serotonin present in platelets using the single particle collision method. For this, an appropriately sized microelectrode, buffer system, and time-current curves are used. When platelets collide with the microelectrodes, the serotonin oxidation current can be detected. This signal can be used to quantify the concentration of serotonin in platelets [2].

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P1.046 Controllable Synthesis of Pt Nanoparticles Encapsulated Inside Dendrimers as Tunable Oxidase Mimics for Spatially Resolved Measurement of Oxygen

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Here, we report strategies for controllable synthesis and 3-dimensional structural analysis of dendrimer-encapsulated Pt nanoparticle (Pt DENs). The controllable synthesis strategy utilizes repetitively coupled galvanic exchange and chemical reduction reactions, which allows the expansion of the applicable number of Pt atoms encapsulated inside dendrimers to more than 1000 without being limited by the fixed number of complexation sites for Pt2+ precursor ions in the dendrimers.[1] 3-Dimensional transmission electron microscopy (3-D TEM) can be applied to reveal the structural characteristics of the whole organic-inorganic hybrid nanostructure of the resulting Pt DENs.[2] The structural analysis reveals the fairly controllable and uniform sizes of the Pt DENs with sub-nanometer accuracy in the expanded size range. In addition, we present a detailed investigation on the oxidase-mimetic activity of the Pt DENs.[3] Importantly, after clarifying intrinsic oxidase-mimetic activity of the Pt DENs, we present simple yet effective approaches for analytical applications, especially spatially resolved imaging of oxygen.[3-5]

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P1.047 Enhancing the peroxidase-like activity of iron oxide nanoparticles by surface functionalization with polysaccharides and its analytical applications

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The peroxidase (POD)-like activity of iron oxide nanoparticles (IONPs) has been utilized in a range of analytical applications. The catalytic activity of IONPs are heavily influenced by the affinity of substrates to the active sites on the surface of IONPs. In this study, we employed three polysaccharides, such as dextran, hyaluronic acid, and chitosan, for surface modification of IONPs and carried out in-depth investigation to elucidate the effect of surface functionalities on the POD-like activity of IONPs. The affinity of substrates to the catalytic site of IONPs was found to be determined by the surface functional groups and hydration layer of polysaccharide coating on the surface of IONPs. The role of hydration layer was further confirmed by the results that the POD-like activity of IONPs coated with a certain polysaccharide having higher water holding capacity was significantly enhanced by salting-out reagent, such as ammonium chloride that is known to reduce the thickness of hydration layer. Moreover, the excellent catalytic activity of dextran-coated IONPs was successfully applied to develop a highly sensitive sensing system for the detection of glutathione (GSH) with a limit of detection of 2.3 nM.

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P1.049 A novel personal glucose meter-based method for miRNA detection by utilizing peroxidase mimicking DNAzyme

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We herein developed a novel personal glucose meter (PGM) based method for miRNA detection by utilizing peroxidase mimicking DNAzyme. The target miRNA in a sample binds to the downstream target binding region of target recognition probe (TRP) employed in this work, which would then serve as a primer and promote the continuously repeated nicking and extension reaction, consequently producing G triplex trimer (G3 trimer) amplicons. The G3 trimer would bind to the exponential amplification reaction (EXPAR) template probe (ETP) and promote the conventional EXPAR, producing a large amount of G3 trimers. The peroxidase mimicking activity possessed by the G3 trimer promotes the oxidation of ferrocyanide ([Fe(CN)6]4-) to ([Fe(CN)6]3-) in the presence of hydrogen peroxide. As a consequence, the amount of [Fe(CN)6]4- responsible for the production of the PGM signal would decrease and accordingly decrease the final PGM signal. Based on this unique design principle, the model target let 7a miRNA was successfully detected down to 2.49 fM with excellent specificity. This work would serve as a promising point-of-care miRNA detection by taking advantage of a very convenient PGM.

P1.050 Inverted polymer solar cell device using various ZnO interfacial layer

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Recently, research on polymer solar cells has been actively conducted to improve power conversion efficiency through the development of new device structures, synthesis of polymer materials and applied to charge extraction layer. This study applies various ZnO thin films (sol-gel process based on high and low temperature and nanoparticle process) as electron extraction layer in inverted polymer solar cells based on PBDB-T:ITIC, and the correlation between ZnO and solar cell performance was analyzed. When the ZnO thin film was formed by the high temperature(450°C) sol-gel process, the sheet resistance of ITO electrode was increased up to 5 times. As a result, the power conversion efficiency was low at 4.12%. In the nanoparticle process, butanol-based ZnO has better dispersion and surface properties than IPA-based ZnO, resulting in improved polymer solar cell performance (PCE of 6.35% and 4.58% with butanol and IPA-based ZnO respectively). In addition, ZnO precursor solution with a low-temperature (150°C) sol-gel process was developed, and as a result of applying it as an electron extraction layer of an inverted polymer solar cell, the device performance was greatly improved (PCE of 8.89%). The main reason for the improvement of the device performance is that the ripple-shaped surface is formed, which facilitates extraction of electrons and has excellent surface roughness.

P1.051 Lanthanide-Based Supramolecular Materials

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Developing functional supramolecular materials from simple building blocks is an active area of research. To this end, the use of f-metal ions to direct the synthesis of complex organic ligands via self-assembly has become a popular method whereby the interesting photophysical properties of the lanthanides can be exploited, alongside any additional functionality built into the ligands. Ln(III)-based materials have applications that include light emitting devices, solar wave-guides and molecular sensors.[1] By adopting a self-assembly approach these systems often show easy processability via solution-based immobilisation methods, including Langmuir-Blodgett deposition, Spin-Coating and Rapid Annealing Self-Solution-Shearing (RASSS) deposition.[2] This presentation will focus on our recent efforts to develop novel 2,6-pyridinedicarbonyl based ligands that can be readily functionalized using 1,2,3-triazole "click" chemistry.[3] Using this approach, we have developed systems that assemble around lanthanide ions (typically we use the luminescent Tb(III) and Eu(III) ions) and then further assemble into more complex systems/materials. Our recent work into developing multi-emissive (dual, triple and quadruple emissive) ultra-thin films prepared using Langmuir-based techniques, white emissive/colour-tunable films and lanthanide-based interlocked architectures (i.e. quasi-branched-[4]-rotaxanes) will be discussed.[4,5]

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P1.052 Organic silicon? Towards single component organic solar cells.

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Since the advent of organic electronics, it has been believed that optically generated excitons within organic materials are so strongly coloumbically bound that a driving force must be present in order to generate free charges. This driving force is created by blending two or more organic materials together to create a bulk heterojunction wherein the two components have complimentary energy levels that facilitate the separation of electrons and holes. However, very recently it has been reported that the state of the art non-fullerene 'acceptor' Y6 indeed shows intrinsic charge generation[1]. This finding has opened up the avenue of treating Y6 akin to a conventional n-type inorganic semiconductor. Moreover, this finding allows us to steer clear of the complicated bulk heterojunction, and optimize fundamental device physics in the simplest architecture of a homojunction. Hence, we have applied the conventional doping strategy to Y6 using a newly developed p-dopant and have received promising results. So far, we have optically characterised thin films of neat and doped Y6, studied the fluence dependence of their photoluminescence, and performed the same measurements on annealed films. We have also made devices with doped Y6 that show improved PCEs relative to neat Y6.

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P1.056 A simple and label-free strategy for creatine kinase assay on a personal glucose meter

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We herein developed a simple and label-free method to determine the creatine kinase (CK) activity by employing the personal glucose meter (PGM) as a detection device. This method relies on the target-induced consumption of glucose by cascade enzymatic reaction (CER) promoted by the combined activities of CK and hexokinase (HK). The target CK induces phosphorylation of adenosine 5'-diphosphate (ADP) to adenosine 5'-triphosphate (ATP) using creatine phosphate (CP) as a phosphate donor. HK then catalyzes the phosphorylation of glucose to glucose-6-phosphate by converting the produced ATP to ADP, which would enter another cycle of CER to further consume glucose in a sample. As a consequence, the glucose level would decrease depending on the CK activity, which could be very conveniently detected on a PGM. With this unique design principle, we successfully determined the CK activity down to 0.0147 U/mL with high specificity against various non-target enzymes. We also verified that the developed strategy can reliably detect CK activity in a heterogeneous human blood sample, ensuring its robust utility in various clinical applications.

P1.057 Preparation of Highly Stable Perovskite Quantum Dots and Light-Emitting Diode Applications

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Perovskite quantum dots (QDs) have attracted lots of attention as next generation display materials due to due to their outstanding opto-electrical properties. However, poor stability under environmental conditions must be solved for commercialization. In this work, perovskite QDs with high structural stability were prepared by introducing (1) UV-crosslinking ligand[1], (2) core-shell structure[2] and (3) alkali metal doping. The structural instability for perovskite QDs are significantly enhanced by preventing ligand dissociation and defect generation.[3]

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P1.058 The use of DHM nano-profilometry to inform the design and manufacturing of a MEMS-based medical implant

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Microelectromechanical systems (MEMS) are miniaturized devices that can be manufactured at scale using commercial processes borrowed from integrated circuit fabrication. This technique allows for high precision and scalable manufacturing which is well suited for fabricating small medical implants. As components are miniaturised, typical characterisation methods and mechanical models need to be adapted to the nanoscale. Modern MEMS transducers have reported sensitivity to a displacement of 1 Å (Apigo, 2016) when averaging over an entire transduction surface. However, the loss of spatial detail limits the ability to investigate the mechanical nature of the sensor. We propose the surface shape of a transducer can be measured to investigate transient behaviour and performance changes over time.

We present a case wherein the novel use of Digital Holographic Microscopy (DHM) (Cuche, 1999) was used to characterise the nanoscale response of the transduction element of a sensor fabricated on the exterior of a medical implant. Early designs exhibited an undesirable hysteresis relating to an unexplained relaxation response. We hypothesized that this was due to the slow, nanoscale release of surface forces acting between manufactured layers. This effect was observed using DHM and led to manufacturing improvements to eliminate the relaxation source in the sensor.

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P1.059 Ultrafast photoexcitation dynamics of organic photodetector

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The optoelectronic properties of organic semiconductors (OSCs) enable their applications in a variety of devices, including organic light-emitting diodes[1], organic photovoltaic solar cells[2], and organic photodetectors (OPDs)[3]. In particular, the inherent advantages in OPD, such as low dark current density, high sensitivity, broad spectrum, and fast response, can be attributed to the strong light-matter interactions of OSC and make OPD an emerging candidate for application in, for example, biochemical diagnostics and optical communications. Recently, a high-performance near-infrared (NIR) OPD[4] based on the single-component active layer chloroaluminum phthalocyanine has been reported, featuring a record-high external quantum efficiency of 43% and a 170 dB linear dynamic range. To gain insight into photophysics behind this device, transient absorption/reflection spectroscopies (TAS/TRS) were performed on different OSC layer structures to investigate their ultrafast photoexcitation. Moreover, direct TRS measurement of the OPD under zero bias unveils an ultrafast optical response, which arises from the free carriers generated by exciton dissociation. In addition, TRS is operated on a biased OPD to explore the ultrafast dynamics under operating conditions. Compared with the un-bias device, the device under positive bias arises new broadband positive ΔR/R signal in the NIR region. We assign this spectral feature to the offsetting of electro-absorption by the screening effect from photoexcited free charge carriers. This experiment reveals the ultrafast charge generation in OPD through direct device measurement, and the measurement method may be applied to other optoelectronic materials to study the ultrafast dynamics behind them.

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P1.060 Advanced light source based ultrafast transient spectroscopy system for material characterization

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Ultrafast spectroscopic measurements are extremely powerful for their ability to observe the exceptionally fast dynamics of molecules or even electrons with unprecedented temporal resolution. Such measurements therefore require laser systems with ultrashort pulse durations and preferably wavelength tunability. Existing ultrafast transient absorption systems (TAS) driven by Ti:Sapphire lasers are facing two main problems: first, its low repetition rate leads to relatively high laser noise and slow data acquisition. Secondly, although optical parametric amplifier (OPA) is routinely employed for adjusting the excitation wavelengths, its complicated optical setup and critical crystal phase matching issue makes it unattractive for general users.

Here, we propose a new scheme that combines an advanced light source, multiple plate compression (MPC) [Optica 2014, 1 (6), Opt. Express 2019, 27 (11), Front. Photon 2022, 3 (937622)] and transient absorption spectroscopy (TAS). We generate an intense octave-spanning spectrum from 550 to 980 nm from 190 fs Yb:KGW laser system and compress the pulse down to 3.2 fs. With proper adjustment of two tunable color filters, the excitation bandwidth and central wavelength can be tuned arbitrarily. The spectral density is about 100 times higher as compared to conventional supercontinuum light sources, such as white light bulk crystal and photonic crystal fiber. This MPC-TAS system has been successfully applied for measuring the ultrafast dynamics of advanced materials such as perovskite [Sci. Rep. 2021, 11, (12847)] and Pt complex 4H [Nat. Photonics 2017, 11 (1), 63–68], making it a great candidate as the next-generation optical characterization tool.

P1.061 Optical sensors for superconducting magnet quench protection: optimizing temperature sensitivity in a quasi-continuous fiber Bragg grating array

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Superconducting magnets are a key component of compact fusion energy systems. The superconducting tapes that generate the large magnetic fields operate only at cryogenic temperatures, and must be protected from uncontrolled thermal runaway events, or quenches, that can lead to catastrophic failure. The environment in which the superconducting coils must operate can be described as extreme: cryogenic temperatures, high electromagnetic noise, and high radiation. This leaves few options for condition-monitoring sensors in this environment. Continuous Fiber Bragg Gratings (cFBG) with up to 1000 sensors at the same Bragg wavelength have been shown to be suitable for applications in hotspot detection in superconducting fusion energy magnets.[1]

In this work, we show that a single sensing region after 1000 similar gratings is still detectable, but with limitations that depend on the choice of FBG parameters. By varying the number of FBG sensors and the reflectivity of each sensor, we map out the parameter space to show the optimal parameters for detecting temperature changes of about 10 K, anywhere along the cFBG. The data is supported by simulations based on a transfer-matrix cFBG model.

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P1.062 Using Optical Spectroscopy to Probe the Impact of Atomic Disorder on the Heusler alloy, Co2MnGa

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The exceptional electronic and spintronic properties of magnetic Heusler alloys, which include half-metals and Weyl semi-metals, make them excellent subjects to study for both fundamental interest and for enabling a wide range of device applications. In the last few years, Heusler Co2MnGa, a room-temperature ferromagnetic Weyl semi-metal [1-4], has shown promise for achieving devices from spin caloritronic energy harvesters [5] to efficient electromagnetic wave generators [6]. However, the usefulness of the Heuslers depends on producing materials with the ideal structural ordering of the atoms in the lattice, and there is much not understood about the electronic properties in the presence of disorder. One method to probe the electronic properties is with optical spectroscopy, but again, there are almost no reported investigations of Co2MnGa using this method.

Here, we present the results of an infrared-to-visible optical spectroscopy study of thin films of Co2MnGa. Combined with a determination of the structural ordering from x-ray diffraction, we have investigated near Fermi energy valence and conduction band intra- and inter-band transitions and their dependence on the atomic order. Motivated by band structure calculations, we have modelled our optical spectra with two Drude terms and two Lorentz oscillators assigned to inter-band transitions. The scattering rate of the itinerant carriers increases three-fold with increasing structural disorder, whilst the carrier density to effective mass ratio is unchanged. We have assigned the feature near 1 eV to transitions across the minority spin band gap along the Γ-X direction. We find the energy of this transition is strongly sensitive to the structural order, decreasing rapidly with increasing disorder as extra electronic states fill the minority spin band gap. Our results demonstrate optical spectroscopy is a sensitive way to fingerprint the technologically-relevant near-Fermi level electronic states in Heusler alloys.

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P1.063 Reservoir Computing using Percolating Networks of Nanoparticles

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Reservoir computing (RC) has attracted significant interest as a framework for the implementation of brain-like information processing systems. It has been demonstrated that network topology affects task performance, and in particular, functional advantage has been attributed to small-world connectivity (many local, few global connections) and critical dynamics [1]. Percolating networks of nanoparticles (PNNs) feature an inherent small-world architecture and critical avalanche dynamics [2]. Their fractal topology, combined with the behaviour of memristive tunnel gaps, can provide the rich nonlinear transformations of electrical input signals which are required for in materio RC. Here I will present recent numerical results demonstrating the ability of PNNs to perform classification and time series prediction tasks. Further, the roles of memory, nonlinearity and dynamical richness will be elucidated by comparing the RC performance of PNNs with that of regular array networks.

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P1.064 Observing graphite form through annihilation of screw dislocations

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Synthetic graphite is critical for battery anodes, nuclear reactors, ultra-high modulus carbon fibres and high-quality graphene. However, the high temperatures required to manufacture graphite lead to a high cost. These high temperatures are needed due to the stability of annealable topological defects. These defects can only be removed through a second order phase transition that occurs with a critical temperature of Tc=~2550 K [1]. Many possible defects have been proposed including 5775 ring defects (Dienes or Stone-Thrower-Wales defects) [1], disclinations – fullerene-like or schwarzite-like [2], dislocations [1] or wormholes [3]. However, to date this critical transformation remains without a coherent mechanism that describes which defects are involved and how they transform during this phase transition, limiting our ability to lower the barrier to graphitisation.

In this work, a custom pulsed graphite furnace was used to observe the kinetics of graphitisation in PVC – a classic graphitising carbon [4]. High-resolution transmission electron microscopy and X-ray powder diffraction were used to track the screw dislocations during graphitisation. Finally, molecular dynamics simulations provided insights into how the screws form and anneal during high-temperature treatments. These results provide the first stop-motion film of graphite forming and suggest new opportunities for reducing the cost of graphite synthesis.

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P1.065 Small and Ultra Small Angle Scattering for Nano- and Micro-Structural Characterisation at ACNS, ANSTO

Dr Jitendra Mata[1], Dr Liliana de Campo[1], Dr Elliot Gilbert[1], Dr Robert Knott[1], Dr Anna Sokolova[1], Dr Andrew Whitten[1], Dr Kathleen Wood[1], Dr Chun-Ming Wu[2]
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Small angle X-ray and neutron scattering (SAXS, SANS, ultra-SANS) are versatile techniques for investigating the nanoscale and microscale structure of hard and soft condensed materials such as minerals, alloys, magnetic materials, food, surfactants, polymers, proteins, colloids and emulsions. These techniques have been exceptionally useful for studying complex materials of industrial importance in recent years. The use of small angle scattering (SAS) in combination with traditional techniques offers a unique insight into the structure, size, shape and morphology of materials. Different processes like aggregation, structural transitions, crystallization and phase separation can be directly studied. SAS techniques are well-established for characterisation at the 1 nm to 10 µm length scales, are mostly nondestructive, and particularly useful to study systems, in-situ, and within complex sample environments. The use of deuterated molecules and partial deuteration has also enhanced the applicability of these methods for soft materials using SANS/USANS. We discuss the advantages and limitations of these techniques, and provide examples of recent applications in various areas of science in this talk.

Australia is the home of state-of-the-art reactor-based SANS and USANS instruments known as QUOKKA, BILBY, and KOOKABURRA (at the ACNS, ANSTO). Combining these with on-site lab-based SAXS instrument provides a versatile characterization suite to study complex materials. ANSTO is known for its high class neutron scattering based science, and associated exceptional sample environment options, as well as outstanding deuteration facility.

Reference:

https://www.ansto.gov.au/research/facilities/australian-centre-for-neutron-scattering

P1.066 Raman imaging of vaterite inclusions in fish otoliths

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Within the inner ear of bony fishes is a calcareous structure called an otolith, usually consisting of aragonite (a polymorph of calcium carbonate).[1] The presence of vaterite (an abnormal polymorph) in fish otoliths has been shown to cause hearing impairment in fish and can be detrimental to their survival, as well as contributing to navigation problems.[2] It has been hypothesized that changes in this calcium carbonate structure also influence the shape and size of the otolith, with vaterite formation resulting in deformation of the otolith.

Scanning electron microscope images were used to distinguish normal from deformed otoliths. A Horiba confocal Raman microscope was then used to map the calcium carbonate polymorph on the inner surface of fish otoliths and found that some indicate significant zones of vaterite. The extent of these vaterite inclusions may play a role in deformation of the otoliths and hence affect the ease at which these fish fall prey to predators.

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P1.067 Synthesis of Hofmann-based metal-organic frameworks incorporating pyrazole linkers, for various gas separations

Miss Brooke Matthews[1,2], Nathan Harvey-Reid[1,2], Victoria-Jayne Scott[2,3], Matthew Polson[1], Ravichandar Babarao[4], Shane Telfer[2,3], Paul Kruger[1,2]

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The design of novel porous materials for gas adsorption and separation is an important focus for materials research. Porous materials that demonstrate selectivity towards industrially relevant hydrocarbon gas mixtures are particularly important, with petrochemical separations currently accounting for the largest portion of the energy consumption of the chemical industry.1

A sub-class of metal-organic framework, hybrid ultramicroporous materials (HUMs) show promise for selecting between relevant hydrocarbon gas mixtures.2 These materials are composed of both organic and inorganic components and have pore diameters of less than 7 Å. Within this class of materials, Hofmann-based metal-organic frameworks are good candidates to study for these separations. These materials are characterised as either 2D or 3D coordination polymers whose frameworks are constructed using cyano-bridged bimetallic layers, pillared by heterocyclic ligands with N-donor atoms.3 Prior research into these frameworks have found they have the potential for high selectivity within hydrocarbon gas mixtures.4,5 Particular selectivity has been demonstrated for C2H2 over other C2 hydrocarbons and CO2 by nature of strong “sandwich-binding” of the C2H2 between two open metal sites from the cyano component.4

Our research considered variations on these frameworks using a range of different transition metal nodes with an N-donor pyrazole-based pillaring ligand to generate isostructural porous frameworks which were then assessed for their uptake ability for a range of gases. Using these uptakes, estimations of their selectivity for particular guests in industrially relevant binary gas mixtures were calculated to determine the potential of the material to carry out that separation in situ.

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P1.068 Development of Portable Raman Spectroscopy as a Clinic Tool for Assessing Photodamage in Skin

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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 developing low cost, portable Raman as a clinical tool to rapidly assess biochemical markers of actinic aging in skin.

Raman spectra from both sun-exposed skin regions (forehead, cheek, forearm, hand, and shin) and sun-protected regions (behind the ear, and underarms) were measured in 119 participants aged four to ninety-four years old. PCA (principal component analysis) and ASCA (Analysis of Variance/Simultaneous Component Analysis) was performed on the resulting data set to identify spectral regions that differentiate photoprotected and photoexposed areas. PLS (partial least squares) regression was also performed on the data to identify spectral regions which correlate with age.

With the existing dataset, spectral regions have already been identified that differentiate young skin from old, and photoprotected from photoexposed. The objective is to find spectral regions, resolvable with the portable spectrometer, that correlate with age for photoexposed regions but not photoprotected regions. These markers will be indicative of actinic damage in skin.

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P1.069 3D printing of flax shives conjugated to fluorophores to design 4D pH-responsive biobased materials

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Incorporation of agriculture unused by-products into materials is a relevant strategy to develop sustainable and profitable biobased products while limiting environmental impacts of plastics. In addition, the design of such biomaterials with 3D printing techniques as FDM allow to bring new functionalities. However, the plant material properties and the interactions with the polymeric network are critical to control during the process, from filament production to 3D printing, to obtain a high-quality material.

In this work, flax shives were selectively milled and the used as a starting plant by-product to be grafted to a fluorophore whose fluorescence varies under pH. The resulting fluorescent shives were processed with poly-(butylene-terephthalate) (PBAT) by extrusion to produce a filament reinforced with 10%-wt of flax shives (whose 10% were grafted), which was 3D printed. Extensive microstructural characterization (particle size and shape analysis, X-ray microtomography) demonstrated that flax particles are homogeneously distributed into the 3D printed material. Despite the relatively low content of fluorescent flax shives in the final 3D printed material (1%-wt) and successive heating stages (during extrusion and 3D printing), a strong fluorescent emission could still be measured.

This work paves the way for using flax shives as reinforcements into composites while conferring them fluorescent properties, thus making 4D materials with potential applications as sensors depending on the fluorophore used.

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P1.070 Nanoparticles surface-functionalised with a branched cell penetrating peptide enhances interactions at the nano-bio interface

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Cellular uptake of nanomedicines depends on the surface characteristics at the nano-bio interface. Effective delivery of therapeutic compounds remains limited by our understanding of interactions between drug carriers and the biological interface. Functionalising nanoparticles with cell penetrating peptides (CPPs) enhances cellular uptake, but the impact of CPP architecture on uptake is yet to be explored. Single particle tracking allows direct visualization of how individual nanoparticles interact with cells and so provides a powerful tool to elucidate how CPP architecture influences cell association.

We produced novel, highly-defined poly(lactic-co-glycolic) acid (PLGA) nanoparticles functionalized with CPPs using microfluidics[1]. CPPs of different architectures (short, long linear and branched) were designed for conjugation to PLGA nanoparticles. Single particle tracking was used to follow the dynamic behaviour of individual CPP-tagged nanoparticles at the nano-bio interface by following their spatiotemporal trajectories.

Uniform functionalised nanoparticles were produced using microfluidics (average diameter > 180 nm and a surface charge of between -16 mV and +8 mV, depending on the conjugated CPP). The initial interactions with cells were similar for all CPP-nanoparticle formulations after 2 min. However, after 1 h, functionalisation with branched TAT displayed mobility behaviour that was distinct from the other CPP-tagged nanoparticles. Critically, branched TAT nanoparticles had a higher degree of membrane interaction defined by three diffusional modes[2].

Using single particle tracking provides key insights into the physical behaviour of CPP-tagged nanoparticles with cells that are not possible with traditional ensemble techniques. This information can inform the design of superior nanomedicines for enhanced drug delivery.

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P1.071 Pseudocapacitance of Monolayer MXenes

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The transition to a low-carbon economy based on renewable electrical energy requires new electrical energy storage technologies. One such technology is supercapacitors, which bridge the gap between tradition Li-ion batteries and parallel plate capacitors. MXenes are 2D transition metal carbides, nitrides, and carbon-nitrides that show excellent performance as the active material in supercapacitors. This has been attributed to MXenes very high surface area, electrical conductivity, and the pseudocapacitive response that stores charge on the surface of the MXene.

We have used a unique experimental configuration to measure the pseudocapacitive response of Ti3C2Tx MXene monolayers, isolating the pseudocapacitive signal from 0.3 µm2 regions of monolayer MXene flakes. We measure incredibility high specific gravimetric capacitances of up to 12000 F/g, nearly 50 times greater than anything that has been measured or predicted previously. A careful analysis suggests that the transport of protons across the surface of the MXene sample is driving our incredibly high gravimetric capacitance measurements.

P1.073 Effect of Post-synthesis Processing on the Electrochemical Performance of Y2W3O12 in Lithium-ion Batteries

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Lithium-ion batteries (LIBs) are enabling the revolutionary migration to electric vehicles and also playing a pivotal role in the realisation of grid-scale battery storage. Graphite has been the material of choice for anodes in LIBs with graphite/silicon composites getting more traction in recent times due to much higher theoretical capacities albeit with their own challenges. It is vital to develop advanced novel materials for next-generation LIBs that are energy dense, safer, cheaper, and environmentally friendly.

Here, the electrochemical performance of solid-state synthesised Y2W3O12 is probed as the active anode material in LIBs. The electrodes prepared with as-synthesised Y2W3O12 powder experience a substantial drop in capacity possibly due to the inherently poor conductivities and resultant loss of conduction pathways as the cycling progresses.

In this work, we investigate the impact of facile post-synthesis modifications such as milling and carbon coating on the electrochemical performance in terms of capacity retention during long-term cycling and rate performance. In particular, carbon coating results in significant performance enhancement. At 100 mA/g, initial coulombic efficiency jumped from 35% for the unmilled/uncoated sample to >60% for the carbon-coated samples. Furthermore, the 1st lithiation capacities for all the samples ranged between 600-700 mAh/g. However, differences in 1st delithiation capacities were quite remarkable for as-synthesised (226 mAh/g) and carbon-coated (425 mAh/g) samples. The carbon-coated samples displayed excellent capacity retention at currents as high as 1600 mA/g. Such a facile post-synthesis process can be easily applied to other electrode materials to enhance their electrochemical performance.

P1.074 Microfluidic Models for Spiking Neural Networks

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Microfluidic channels have long shown potential as media for mechanical computation: for example, fluid channels that behave analogously to electronic devices such as logic gates and timers [1] have been known for some time, while more recent work has introduced diode- [2] and field effect transistor-like structures [3]. Meanwhile neuromorphic computing [4], which relies on specialised electronic processors to mimic biological structures, is rapidly extending the bounds of conventional, electronics-based computation. One of the biological structures that has gained special interest is the spiking neural network [5], as it allows great flexibility in the way time-dependent information is encoded.

In this work we aim to explore how droplet microfluidic channels [6] can be extended to mimic the behaviour of spiking neural networks. We present modelled data generated using the Basilisk [7] solver to characterise fundamental microfluidic components such as T-junction droplet generators [8], splitters [6], and mergers [9], before showing how these channels can be combined together to realise the building blocks of artificial neural networks, including spiking neural networks. We also discuss potential uses for these designs, as well as several fundamental limitations.

P1.075 Thermoelectric properties of nanocomposite indium-tin-oxide thin films

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Transparent thermoelectric materials offer synergetic performance for energy harvesting as “smart windows” which could sense the temperature gradient which can be used for energy harvesting waste heat and direct sun light to power the air-conditioning and low power home appliances [1]. The conversion efficiency of the device is dependent on the thermoelectric figure of merit ZT = α2σT/κ of the materials, wherein σ and κ are the electrical and thermal conductivities, and T the absolute temperature. Realizing high ZT is an exacting challenge because it requires strategies to optimize unfavourably interlinked α, σ and κ [2].

We report optical and thermoelectric properties of transparent thermoelectric materials indium-tin-oxide (ITO) films. The ITO films were deposited using ion beam sputtering method at various partial deposition pressures [3]. Oxygen vacancies in non-stoichiometric (In1.8Sn0.2O2.5) films prepared at partial deposition pressures (≤1 × 10−5 mbar) aided the formation of In-rich metallic clusters [4]. Hall results showed the highest electrical conductivity (σ = 1540 Scm−1) and Seebeck coefficient |α| = 27.2 μVK−1, which resulted in the highest power factor (α2σ = 113.8 μW m−1K−2) but low optical transmission (~25%). An increase in oxygen partial pressure resulted in stochiometric In1.8Sn0.2O3 films which improved the optical transparency by 3 times (75.4%) but decrease in power factor. Our results showed that defects play a crucial role for obtaining highly transparent and efficient power factor in nanocomposite films. The results based on optical, compositional, structural, electrical and thermopower measurements on ITO films will be presented in detail at the conference.

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P1.076 NaMgF3:Ln (Ln = Eu, Sm) nanoparticles sensitisation using 2-thenoyltrifluoroacetone

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Lanthanide (Ln)-doped materials have been extensively researched for application in devices for sensing, solid-state lighting and displays (1) since they exhibit unique luminescent properties and emit in various spectral regions. However, Ln3+-ions such as Sm3+ display low luminescence signals due to the low oscillator strengths of their parity-forbidden intraconfigurational 4f-4f transitions (1, 2). Therefore, the functionalisation of such materials is vital to increase their luminescence signals. Co-doping such ions with ions which have allowed 4f-5d transitions may result in the energy transfer between the ions. For example, Ce3+ → Sm3+ energy transfer was reported in NaMgF3:Ce,Sm and other compounds (2-4). Furthermore, sensitising ligands may additionally be attached to the nanoparticles, where excitation of the ligand results in energy transfer to the Ln-ion via an "antenna effect" (1, 5). Ln-ion sensitisation has been demonstrated in similar materials by attaching 2-thenoyltrifluoroacetone (TTFA) on LaF3:Eu and LaOF:Eu nanoparticles (5, 6). The energy transfer process is widely reported in the literature and is governed by several factors, including the energy difference between the ligand triplet state and the Ln-ion resonance energy level (1).
Herein, we report on the luminescence properties of NaMgF3:Ln (Ln = Eu, Sm) nanoparticles before and after ligand exchange using TTFA. Remarkable TTFA → Eu3+ sensitisation was demonstrated, rendering the nanoparticles suitable for radiation and temperature sensing. However, minimal TTFA → Sm3+ sensitisation was observed, attributable to a non-optimal energy difference between the TTFA triplet and Sm3+ resonance energy states. Schematic models are presented to explain this discrepancy.

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P1.078 Machine learning for metal-organic framework-based chemiresistive sensor

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Metal oxides are widely used as chemiresistive sensors due to their high sensitivity and fast response, however, their selectivity towards different chemicals is often poor. In this presentation, we present recent efforts to develop non-contact chemiresistive sensors which combine the metal oxide TiO2 with metal-organic frameworks. Importantly, our chemiresistive sensor is found to have dramatically improved selectivity towards certain explosive molecules due to the selective absorbance properties of the metal-organic framework. We have also used density functional theory to reveal the new electronic properties of our sensor and are developing a machine learning model to optimise sensor performance.

P1.079 Functionalisation of Ethene via an Aluminacyclopropane

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The non-reversible carbonylation of ethene has been established utilising the potassium aluminyl, $[K\{Al(NONDipp)\}]^{2-}$ ($[NONDipp]^{2-}$ = $[O\{SiMe_2NDipp\}_2]^{2-}$, Dipp=2,6-$iPr_2C_6H_3$).[1] With the latter class of chemistry being largely dominated by transition metals, the expansion to main group systems suggests scope for their employment in sustainable small molecule activation with synthetic utility.

This work examines the introduction of various substrates into the aluminacyclopropane complex to afford ring expanded products in high yields under mild reaction conditions. Thermally induced retro-Brook rearrangement of the diamidosilylether backbone in K[Al(NONDipp)(κC,N-$CH_2CH_2C\{=NiPr\}NiPr$)] affords K[Al(NNODipp)(κC,N-$CH_2CH_2C\{=NiPr\}NiPr$)]. The rearrangement grants access to electronically non-symmetrical reaction sites around the Al centre increasing scope for further insertion chemistry and chain extension.

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P1.080 Development of a serum-free suspension culture system for scalable production of bovine satellite cells for cultured meat

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Cultured meat holds great potential in the meat industry as it is a more sustainable, ethical, resilient and healthy food system compared to traditional meat. Cultured meat is primarily composed of skeletal muscle fibres, which are derived from muscle satellite cells. Standard protocols for growing cultured meat require an expansion of muscle satellite cells in adherent two-dimensional (2D) cultures under high fetal bovine serum (FBS) conditions, followed by myogenic differentiation through a drastic reduction in serum concentration. However, to become commercially viable, the cultured meat industry must overcome two major challenges: 1) dependence on FBS, which is a notoriously expansive and inconsistent component, during cell expansion and 2) inability to expand muscle satellite cells in suspension culture system that provides scalability. In our project, we will generate bovine muscle satellite cell lines from New Zealand cattle (Bos taurus), following the standard isolation protocol performed in 2D culture under high FBS conditions. The cell lines will be characterised for satellite cell marker expression and myogenic potential. Depending on the heterogeneity of cell population, purification steps for satellite cells may also be required. Next, we will test various chemical factors and microcarriers coated with different materials to integrate a serum-free suspension culture system for bovine satellite cells. Transcriptomic analysis using single-cell RNA sequencing (e.g., comparing cells cultured in the presence or absence of FBS) will also be an option for more targeted approach. This work will offer a foundation for the cultured meat industry in New Zealand, thereby accelerating the sector.

P1.081 High rate deposition of oxide semiconducting films using hot hollow cathode discharge

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In this work, we present a plasma deposition technique that allows the reactive deposition of oxide layers with an extremely high deposition rate. The new approach combines reactive sputtering by DC hollow cathode discharge with thermal evaporation from the hot surface of the hollow cathode. As examples of successful fast deposition, photoactive films of titanium dioxide (TiO_2) [1,2], cobalt oxide catalysts (Co_3O_4) [3], and non-stoichiometric tungsten oxides films (WO3-x, $0 < x < 3$) [4] with various thicknesses, were deposited using this technique. The uncooled Ti/Co/W nozzles served as hot hollow cathodes and simultaneously as an inert gas (Ar) inlet. The reactive gas (O_2) was introduced into the vacuum chamber through a separate inlet. During deposition, the temperature of the hollow cathode reached up to 1600 °C, depending on the nozzle material and discharge parameters. This made it possible to combine the ion sputtering of a hot metallic cathode with its thermal surface evaporation, which significantly increased the deposition rate of the final oxide structure. The highest achieved deposition rate for TiO_2 was 567 nm/min (34 µm/h), which (with respect to the geometry of this process) corresponds to total volume of the deposited TiO_2 material 1.2 mm^3/min per 1 kW of absorbed power. Despite extremely high thermal flux to the substrate, TiO_2, Co_3O_4, and WO_3 films were successfully deposited even on temperature-sensitive PET foil.

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P1.082 Multi-component MOFs as modular heterogeneous asymmetric catalysts

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Asymmetric catalysis is a type of targeted synthesis in which a chiral catalyst directs the formation of a chiral compound such that one particular stereoisomer is the favoured product. Since the catalyst is not consumed in this process, it may be used in a sub-stoichiometric quantity, potentially improving efficiency and avoiding waste. This type of selective synthesis finds important applications in the production of most pharmaceuticals, fabrics, flavours and green chemistry.[1] To this end, Telfer and co-workers have been investigating asymmetric catalysis using metallo-organic frameworks (MOFs),[2] which are 3-dimensional coordination compounds made of metal clusters and organic ligands. These crystalline materials are often highly porous (can be seen as molecular 'sponges'), and can allow for chemical reactions to take place within their pores.[3] This project aims at using asymmetric catalysis by carefully including individual chiral and catalytic functional groups into the building blocks of crystalline MOFs using a modular approach. A range of important organic reactions (e.g., aldol, Friedel-Crafts, Henry) are performed heterogeneously in the presence of these MOFs in order to induce high enantiomeric selectivity, thus introducing a new way to perform asymmetric catalysis.

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P1.085 A New Design for Asymmetric Catalysts

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Catalysis rules the chemical kingdom with asymmetric catalysis occupying the throne.1 Asymmetric catalysts produce chiral molecules: mirror-image molecules akin to your hands (enantiomers). To enable the transfer of chiral information from the catalyst to the reaction substrates, asymmetric catalysts are themselves chiral.2 In typical asymmetric catalysts, the catalytic and chiral motifs are held close together.3 We are breaking this mold with a strategy we call 'remote asymmetric induction' (RAI). In RAI catalysts, the catalytic and chiral motifs are independent. To design catalysts in this way we draw on a set of materials known as multicomponent metal-organic frameworks (MOFs).4 The catalytic and chiral motifs are individually anchored to different building blocks of these MOFs, and they define a spatially confined active site in the frameworks. I will outline our proof-of-concept experiments and chart the way forward to highly enantioselective catalysts.

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P1.086 Recyclable sulfur polymers synthesised by electrochemical induced ring opening polymerisation

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In recent years sulfur polymers produced by inverse vulcanisation have shown a variety of capabilities in solvent resistant coatings,1 heavy metal remediation,2 and IR thermal imaging3. In order to tune the properties of the sulfur-based polymers a key area for development is to control their sulfur rank and molecular weight. In this research, cyclic sulfur containing monomers have been used to make sulfur polymers in a controlled fashion by electrochemically induced ring opening polymerisation.4 These same polymers can be thermally depolymerised back to monomer. These finding are significant for improving the current applications of sulfur polymers by providing methods for controlled synthesis. Additionally, the nature of these polymers allows for depolymerisation back to the starting monomer resulting in a fully chemical recycling process.

P1.087 Creation of highly specialised composite hydrogels for modelling of cardiac pathologies.

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The cardiac extracellular matrix (ECM) is a highly complex, hierarchical and anisotropic material that determines cell fate and structure. Creating highly specific hydrogels for 3D cell encapsulation that better mimics its in-vivo counterpart can elicit predictable cell formation, differentiation and protein expression, which can be exploited to mimic particular pathologies [1].

This project proposes a system to create models that mimic the border region between healthy and fibrotic cardiac tissue. This is done by encapsulating induced pluripotent stem cells (IPSC) derived cardiac myocytes and fibroblasts within Gelatin methacryloyl (GelMA) hydrogels cross-linked with a photo initiator. The creation of healthy and fibrotic tissue is done by modulating the stiffness of the encapsulating hydrogel using a digital light processing set-up to control the degree of crosslinking on a micrometre scale. Cardiac tissue stiffness is related to pathologies as cardiac stiffness is highly elevated in fibrotic tissue. Studies have shown that ECM stiffness controls the differentiation of cardiac fibroblasts into their more active myofibroblast state [2]. These myofibroblasts are upregulated in in-vivo fibrotic tissue and are critical to forming cardiac scar tissue.

We will present our findings on both the mechanical properties and resolution of photo-patterned hydrogels, the viability of Cardiac myocytes encapsulated with GelMA, as well as the effect of stiffness on both IPSC-derived cardiac myocytes and fibroblasts and the feasibility of creating accurate cardiac scar models.

This research will further the knowledge on the formation and possible regression of cardiac scar tissue on multiple cell sources.

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P1.091 Elucidating the Dehydration Mechanism of Nitrofurantoin Monohydrate II Using Low-Frequency Raman Spectroscopy

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Raman spectroscopy offer a rapid, non-destructive, and relatively inexpensive method for measuring complex mixtures and systems, with the potential for identification, quantification, classification, and process monitoring of pharmaceutical systems. The low-frequency Raman region (< 300 cm-1) is of particular value to solid state analysis because it probes phonon/intermolecular modes which are extremely sensitive to change in the solid state of compound or system.

Previous report have stated that the popular antibacterial medication, nitrofurantoin, exists in multiple solid-state forms, with at least two hydrates (I and II) and two anhydrous forms (alpha and beta). In this work, we monitor the isothermal dehydration kinetics of nitrofurantoin monohydrate II using Raman spectroscopy contrasting the mid- (300 - 1800 cm-1, intramolecular vibrations) and low-frequency (15 - 300 cm-1, intermolecular vibrations) Raman regions.

P1.092 Synthesis and Reactivity of Lanthanide(II) Hydrides

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The development of trivalent lanthanide hydrido species has experienced impressive growth, so much that this chemistry has now been extended to most f–elements. Their reactivities have become well established in the literature, being found to favor small molecule activation as well as demonstrating high catalytic activity towards a range of chemical transformations.1,2 In contrast, the synthesis and reactivity of lanthanide(II) hydrides is largely underdeveloped and was attributed to the assumption that the larger ionic radii and the strong reducibility of the metal ions posed a challenge in the synthesis and stabilisation of well defined, discrete lanthanide(II) hydrides. It has been illustrated that this assumption is continuously being defied, with the literature disclosing a total of six well-characterised ytterbium(II) hydrido complexes, in which the hydrides are exclusively bound to the metal centre.3,4

In contrast, there have been no reports of the synthesis of a europium(II) hydride in the literature, despite europium being more stable in the 2+ oxidation state compared to ytterbium. This means the lack of reported hydrido species for this element is likely ascribed to the larger ionic radius and the challenge of finding a suitable ligand environment for stability.

We, therefore, aim to synthesise the first example of a molecular europium(II) hydride. As their reactivity remains completely unexplored, it presents a unique opportunity to explore their catalytic abilities for the first time in relation to industrially relevant chemical transformations such as hydroamination, hydroboration, hydrosilylation, hydrogenation, and polymerisation reactions.

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P1.094 Flicking the switch to carbon dioxide reduction by melting metallic alloys

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The electrochemical reduction of carbon dioxide into industrially relevant value-added hydrocarbons is a critical goal for renewable energy and sustainability.[1] Optimising catalysts for electrochemical CO_2 reduction is one route towards carbon-neutral processes, without the need for large areas of fertile land required for organic carbon capture and biofuel production.[2]

The performance of traditional pure-metal catalysts (e.g. Cu, Au) for CO_2 reduction has historically been limited by poor selectivity towards the desired products,[3] arising due to competing electrochemical reactions (hydrogen evolution) and production of unwanted by-products (carbon monoxide).[4] One recent report[5] demonstrated highly promising CO_2 reduction behaviour from a new type of catalyst – a eutectic metal alloy at the solid-liquid phase transition. Ga-Sn and Ga-In catalysts exhibit no CO_2 reduction activity in solid form, but when melted at slightly above room temperature the alloys "switch" to producing formate with >95% efficiency. The structural and/or electronic reasons behind the selectivity switching at the phase-transition remain unclear.

This presentation will discuss our work using ab-initio molecular dynamics simulations to understand the melting behaviour of Ga-Sn and Ga-In. We cover both structural and electronic changes in the materials, and the dynamics in the liquid phase. These properties can be related to changes in the binding strength of intermediates in the CO_2 reduction pathway, and to the mechanisms of interconversion. The results allow us to characterise the features controlling product selectivity on these novel alloy catalysts, and could direct the design of a new class of phase-transition catalyst materials in the future.

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P1.095 On Surface CO2 catalysis: Lanthanide-based coatings for CO2 activation – towards a CO2 economy

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With increasing populations and industrialisation, achieving climate and sustainability goals will require not only an increase in the efficiency and deployment of renewable energy technologies, but also in the capture and storage or utilisation of CO_2. If this CO_2 can be used as a feedstock in chemical industries, we achieve the goal of reducing environmental CO_2 whilst also developing important molecules, such as fuels. To utilise captured CO_2, efficient CO_2 activation catalysts are required which can ideally be deposited onto solid surfaces. Preliminary studies support that lanthanide ions possess the ability to act as CO_2 activation catalysts due to their oxophillic nature [1,2]. Additionally, a subset of 1,8-napthalimide ligands have been reported to have the ability to form layered systems on surfaces [3,4]. Thus, our research aims to answer the question "can on-surface lanthanide networks act as CO_2 activation catalysts/materials?". Throughout this presentation, results surrounding our progress in achieving this aim are presented. In particular, results surrounding the synthesis and characterisation of a family of naphthalimide-sulfonate ligands are presented [4]. Additionally, the ability of these ligands to self-assemble with lanthanide ions to form complexes and metal-organic frameworks (MOFs) will be presented. Lastly, preliminary studies regarding the surface immobilisation of these complexes/MOFs along with the testing of these systems for CO_2 activation/reduction will be presented.

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P1.096 Optical temperature sensing using sensitised nanoparticles: Thermal quenching of the Ln3+ luminescence in NaMgF3:Ln,TTFA

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Non-electrical temperature sensors are urgently needed for applications in hazardous environments (e.g., high voltages, explosive and corrosive chemicals). Optics-based sensors are an ideal solution where, for example, the luminescence of compounds attached to an optical fibre can be used to measure the temperature[1]. However, the luminescence intensities are low and this limits the temperature resolution. One method to increase the intensities is to use nanoparticles with optically sensitised surfaces[2]. The use of nanoparticles can also lead to high spatial resolution sensors due to reduced light scattering[3]. Therefore, it is of interest to investigate new sensitised nanocrystalline luminescent compounds as novel luminescent nanothermometers.

We present the results of luminescence studies on 2-thenoyltrifluoroacetone (TTFA)-sensitised $NaMgF_3$:Ln nanoparticles. We show that the incorporation of TTFA sensitises the luminescence of Ln3+ ions, such that the luminescence intensities are increased by several orders of magnitude relative to those achieved via conventional 4fn → 4fn stimulation. Moreover, the energy transfer TTFA → Ln3+ exhibits a strong thermal dependence, where the luminescence intensities decrease with increasing temperature. We present a model describing these results, where the rate of energy transfer depends on the energy difference between the triplet state of the TTFA ligand and the resonant 4fn level of the Ln ion, and the thermal quenching depends on the rate of back-transfer. Via careful selection of the Ln dopant, the thermal quenching properties can be optimised for specific temperature ranges. Ultimately, we aim to show that the nanoparticles can be used to construct reliable non-contact optical temperature sensors.

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P1.097 Application of RuO2-based materials as oxygen evolution catalysts in a PEM water electrolyser

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Developing sustainable and green energy technology is one of the primary goals of the scientific community to address the increasing global energy demand and fossil fuel-related climate issues. In this regard, hydrogen produced from renewable energy-driven water splitting is ideal for future large-scale and long-term renewable energy storage. In a typical water electrolyser, the hydrogen evolution reaction (HER) is complemented by oxygen evolution reaction (OER) at the anode. OER is a kinetically sluggish reaction compared to HER and thus requires more overpotential and is generally carried out in extreme conditions [1].

Today, IrO2 and RuO2-based materials dominate the catalysts for OER due to their excellent catalytic properties. However, the high cost of these materials, especially iridium, questions the economic translation of technology on an industrial scale. Recent theoretical and experimental studies have shown that doping RuO2 with transition metals can increase its activity, provide stability to the binary oxide, and reduce material cost [2, 3].

In this work, we synthesised and studied 3d-transition metal-doped RuO2 nanoparticles for OER. The electronic and structural properties of nanomaterials were obtained using X-ray diffraction, X-ray photoelectron spectroscopy, and transmission electron microscopy. The OER electrocatalytic activity of these materials was accessed in 0.5 M H2SO4 and a PEM electrolyser. Overall, the best cell voltage we achieved was 1.6 V at 1 A/cm2 at 80 °C and using the Nafion115 membrane. The stability of doped materials was studied by observing the change in composition and electronic properties of the electrode material using XRD, XPS, and ICPMS.

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P1.098 Superalkalis: catalysts for carbon dioxide activation

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Superalkalis are clusters of atoms that act like a single atom. They have unique properties, including diverse functionalization, redox activity, and magnetic ordering. Materials made up of superatoms, so-called cluster-assembled solids, hold the promise of high tunability, atomic precision, and robust architectures. Superalkalis are a class of superatoms that have extremely low ionization energy and might serve as catalysts. Carbon dioxide (CO2) is a major greenhouse gas, yet is a cheap carbon feedstock. Developing efficient catalysts that convert CO2 into fuel is vital to addressing the energy crisis and global warming. The high stability of CO2 makes the conversion difficult. We design and explore superatoms for CO2 activation and transformation, using computational chemistry with quantum chemistry techniques. We investigate the influence of electronic structure, ionization energy, and ligation on the stability and selectivity of superalkali/carbon dioxide complexes. We believe that our results will enhance our understanding of CO2 conversion into fuels and value-added chemicals. Subsequently, this can be used to develop a pathway for sustainable carbon dioxide utilization and global warming reduction.

P1.099 Strategic Hydrometallurgical Processes for End-of-Life photovoltaics to achieve different outcomes

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Photovoltaics (PV) has been emerging as one of the promising green energy technologies. The PV industry has since thrived and is expecting to record a global cumulative PV capacity of 1,600 GW in 2030 and 4,500 GW in 2050 [1]. Although the typical lifespan of a PV panel is approximately 25-30 years, it is crucial that proper waste management is in place to deal with the projected influx of end-of-life (EoL) PV in the near future. Valuable materials such as high purity silicon and silver can be recovered from these wastes and further upcycled to high-value materials. Conventionally, the hydrometallurgical approach employed widely stems to dissolve all the metals present, followed by metal separation techniques such as precipitation and lixiviant encapsulation to isolate the desired metal ions before recovering the raw materials as their elemental or compound forms. This in a way wasted the chemical utilised in the leaching step as meticulous planning can allow selective dissolution of metals by employing strategic reagents and thereby minimizing chemicals wastage. Herein, we present various proposed hydrometallurgical approaches to achieve different objectives in the PV recycling and how these approaches pave the way to recovery or upcycling applications [2-4].

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P1.100 Fluorescent Colorants With Rigid Molecular Structures To Enhance Light Stability Functions

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In this study, novel type of fluorescent compounds with rigid molecular structures were prepared and characterized by spectrophotometric studies. The photochemical functions (UV radiation) of these compounds were discussed in liquid medium. Compared to that of a commercially available molecule, the prepared colorants displayed improved photostability behaviors in these solvents. A coloration experiment was also carried out on modacrylic polymer with these compounds with a traditional coloration method. The coloration results exhibited that all the developed high visibility molecules showed clear fluorescence effects.

With regards to the luminance factor and photostability characteristics, the designed and prepared colorants can be used in high visibility purpose, fluorescent function and warning end-uses with enhanced light stability [1,2].

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P1.101 Electrochemical Ammonia Production: Challenges and Promises

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Reactive nitrogen in the form of ammonia directly sustains half of the global population. However, ammonia production by the Haber Bosch method is energy and capital-intensive resulting in 450 Mt of CO2 emissions every year[1]. Over-utilisation of ammonia in the form of fertilisers has led to dangerous altercations in the elemental nitrogen cycle (nitrous oxide emissions and nitrate leaching). Renewable-powered electrochemical nitrogen reduction (eNRR) offers a promising pathway to realise green, distributed generation of ammonia from just air and water. Implementing this technology directly at farms will enable calibrated utilisation of ammonia, significantly reducing their nitrogen emissions. Most important of all, eNRR paves way for use of ammonia as a viable energy carrier. With its high volumetric energy density, ammonia is the most promising zero-carbon energy vector for long-term energy storage and large-distance transport[2].

This talk will provide a brief overview on the present status and global targets for green ammonia production. The fundamental origin of the four core-challenges restricting eNRR, namely – dinitrogen activation, selectivity, scaling relationships and solubility will be discussed. Our recent progress in developing novel eNRR catalysts based on transition metal nitrides and single atom catalysts will be covered. We will also discuss the practical challenges in measuring eNRR[3]. In this regard, we have developed a lab-scale reactor powered and controlled by a potentiostat. The setup is coupled to an ion chromatography system that allows ammonia quantification in ppb levels. The results from these studies will be presented along with a discussion of future opportunities.

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P1.102 Holey Moley: Toward 3D Covalent Organic Frameworks

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Covalent organic frameworks (COFs) are an emerging class of porous materials which have the potential to front a new wave of environmental and energy technologies. Using principles of reticular chemistry, COFs are synthesized via precise covalent bonding of organic monomers to build highly porous and highly structured networks akin to a 'molecular sponge'. Compared to other porous materials, COFs hold the unique benefits of ordered structures and high stability. Their large surface areas, modifiable pore walls, accessible pore systems, and highly ordered structure make COFs ideal for applications in gas storage, capture and filtration, catalysis, sensing, and optoelectronics. While 2-dimensional COFs have been widely studied, 3-dimensional COFs eliminate many of the drawbacks of their 2D counterparts. Further progression of new 3D COF design may be the push needed to commercialize this porous material into a range of applications. This presentation discusses the progress of a Master's project focusing on the design and synthesis of a series of new covalent organic frameworks.

P1.103 Synthesis and Reactivity of the Indyl Anion

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Group 13 metals exist in the +3-oxidation state due to having 3 electrons in the outer most shell. Over the past two decades research into synthesising these metals in the +1-oxidation state has been extensively explored.1 To ensure stability of anionic metal complexes N-heterocyclic ligand systems have been used. The σ-electron withdrawing and π-electron donating characteristics of the nitrogen atoms of these N-heterocyclic systems help stabilise the anionic compounds. Major work has been focused on the synthesis and reactivity of gallium, boron and aluminium anions utilising these N-heterocyclic ligands.1.2.3 However, all these compounds are neutral. The implications of synthesising these anionic compounds have shown vast interest in small molecule activation and exploring the formation of new metal-metal bonds.
In contrast, the research conducted on the indium anion is not as extensive. However, landmark discovery and the only reported indyl anion was published in literature in 2018 by Anker and colleagues.4 Therefore, my research aims to expand on the synthesis, structure and reactivity of new stable indium anions. This will be achieved through developing new ligand systems and alternate synthetic methods. To date we have synthesized two new indyl anions which have shown to activate and functionalise CO2.

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P1.104 Flutamide-loaded nanostructured lipid carrier exhibits its male contraceptive effects by disrupting blood-testis barrier

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The blood-testis barrier is a complex reproductive structure, which is extremely important for male fertility[1]. Thus, interrupting blood-testis barrier can be an excellent strategy to develop the non-surgical castration for male animals. Administration of flutamide, an antagonist of testosterone, is reported to weaken the blood-testis barrier[2]. However, the use of flutamide as a male contraceptive agent remains challenging mainly due to its poor bioavailability[3]. Here, the flutamide-loaded nanostructure lipid carrier (FLT-NLC) was synthesized, and its antifertility effects were demonstrated by an in vitro blood-testis barrier model. The flutamide was incorporated into the nanostructure lipid carrier by a homogenization method resulting in a high encapsulation efficiency (99.7 ± 0.04%). The FLT-NLC was negatively charged (−27.90 ± 0.10 mV), with a nano size (182.13 ± 0.47 nm) and narrow dispersity index (0.17 ± 0.01). An in vitro release study demonstrated a slower release profile of FLT-NLC when compared with free flutamide suspension (FLT). The FLT-NLC at doses up to 50 µM showed no significant cytotoxic effects against mouse Sertoli cells and fibroblast cells ($p > 0.05$). An in vitro blood-testis barrier with FLT-NLC demonstrated remarkable lower integrity when compared to those with FLT at similar dose ($p < 0.01$). Moreover, FLT-NLC significantly decreased the mRNA expression of blood-testis barrier proteins, CLDN11, while FLT at the similar dose failed to do so. In conclusion, we successfully synthesized FLT-NLC and confirmed its superior antifertility effects on in vitro blood-testis barrier over FLT, indicating the possible application of FLT-NLC as nonsurgical contraception.

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P1.105 Single-Atom Catalysts for Electrochemical Ammonia Production

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Electrochemical nitrogen reduction reaction (eNRR) under ambient conditions is emerging as a promising, sustainable alternative to the energy- and capital-intensive Haber–Bosch ammonia production. The sluggish kinetics of eNRR which occurs at similar cathodic potential as hydrogen evolution reaction results in poor Faradaic efficiencies. In addition, the high reaction barrier for N≡N bond splitting severely restricts their production rate. Achieving both high ammonia production rate and faradaic efficiency, therefore requires electrocatalysts with high selectivity towards N_2 and a sufficient activity towards nitrogen reduction at low overpotentials [1,2].

Single-atom catalysts (SACs), with atomically isolated metal active sites dispersed on supports, have attracted tremendous interest in electrocatalysis. Owing to their maximum metal utilization efficiency, SACs usually show high conversion rates. The homogeneity and tunable coordination environment of the active sites enable high selectivity for a range of electrochemical processes [3]. However, the high surface free energy resulting from the atomic nature of the active sites leads to metal aggregation reducing their utilisation efficiency.

This project focuses on fabrication of transition metal SACs on N-doped carbon derived from zeolite imidazolate framework carbonization for eNRR. The high surface area, high porosity, and abundant N species of N-doped carbon is proposed to anchor the metal atoms leading to enhanced stability. Atomic emission spectroscopy, X-ray diffraction and X-ray photoelectron spectroscopy indicate successful incorporation of metal species on the support. The electrocatalytic performance of the SACs are evaluated in a lab-scale electrochemical reactor using potentiometry. The ammonia production is further quantified by the salicylate method and ion chromatography.

P1.106 New promising materials for efficient nonlinear and ultrafast nanophotonics

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Nonlinear optics on the nanoscale require different prerequisites than on the macroscopic scale. While traditional aspects such as phase-matching and low losses move into the background, a high linear refractive index and the accessibility for common fabrication techniques are crucial for nanophotonic engineering.
Against this background, one promising group for nonlinear applications are Weyl semimetals (WSMs), materials presenting a single touching point of valence and conduction band together with a linear electron dispersion relation. It was shown that this leads to record-values of high second-order susceptibilities[1] and nonlinear optical current generation via the bulk photovoltaic effect[2]. Our work investigates recently realized thin films of the WSM niobium phosphide[3] with respect to its linear and third-order nonlinear optical performance. We show an ultrafast optical response with sub-100 fs relaxation time by nondegenerate pump-probe spectroscopy and efficient third-harmonic generation, that we can attribute to the topological surface states of the material[4].
On the other hand, ferroelectric materials represent a promising material system for second-order nonlinear optics, due to their naturally broken inversion symmetry and nonzero permanent electrical polarization. Here, we present the study of second-harmonic generation (SHG) from nanosheets of the ferroelectric niobium oxide diiodine (NbOI2), reaching an absolute conversion efficiency of 6·10^(-3) %. We show that the efficiency can be scaled with the thickness of the nanosheets, contrarily to other two-dimensional materials, and can be further boosted by the application of mechanical strain or external DC electric fields[5].

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P1.107 Electronic properties on a dense k-grid: Applications of Wannier interpolation to the rare-earth nitrides

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The interpretation of the Kohn-Sham orbitals of the density functional theory (DFT) ground state has yielded a cornucopia of results over the past decades, including representations of the band structure and density of states as well as predicted electronic and structural properties of many materials. This technique has become the workhorse of the computational condensed matter physicist. In recent years, increasingly powerful computers have allowed ever more complex calculations to be performed, however some tasks, such as density of states calculations on large super-cells, are still prohibitively expensive. These problems can be circumvented through the use of Wannier functions, which provide an alternative treatment to the problem than the Kohn-sham orbitals of DFT, whilst being much less computationally expensive. Here we present an initial application of a combined DFT and Wannier function analysis to gadolinium nitride, the central member of the rare-earth nitride series of intrinsic magnetic semiconductors. We describe how DFT ground-state Kohn-Sham orbitals are transformed into maximally-localised Wannier functions, and present band structure and density of states calculations showing that these treatments provide equivalent results in our system. Finally, we compare the calculated and experimental optical conductivity, the agreement of which implies that the calculated band structure accurately represents the material for some eV around the optical band-gap.

P1.109 Structural Studies of Amorphous Systems Using Molecular Dynamics Simulations and X-ray Scattering Experiments: Developing Models for the Carrageenan Disorder-Order Transition

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κ-carrageenan is a sulfated biopolymer whose linear chains self-assemble into a 3D gel network with tunable viscoelasticity [1]. Crucial to this is a salt- and temperature-induced structural change from 'disordered-' to 'ordered-states', for which the various competing models have been difficult to prove due to the amorphicity inherent to such systems [2]. In this study we overcome this difficulty by using molecular dynamics to simulate the structures formed in κ-carrageenan solutions on length scales of ~10 nm and over time scales of ~1 μs. Simulated atomic coordinates are used to compute structurally sensitive observables such as wide-angle x-ray scattering profiles and chiroptical properties, which are then compared to experimental data as a means of validating the molecular models proposed. The experimentally validated model for the disordered-state is that of an extended chain with a loosely helical secondary structure, whereas for the ordered-state the validated model is of a double-helix that forms spontaneously at a rate dependent on salt concentration [3]. Crucially, simulations show that the changes to chains' secondary structure during the disorder-order transition are a consequence of double-helix formation, rather than a prerequisite to it as previously thought [4]. These findings will be important to those designing materials incorporating carrageenan, however the techniques presented here will be of broader interest to anyone seeking structural information for amorphous materials.

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P1.110 Multi-scale modelling of charge carrier dynamics in cluster assemblies

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Assemblies of atomically precise nanoclusters have recently been synthesised to demonstrate the dependence of electronic transport properties on structural order[1]. The nanoclusters themselves are examples of superatomic species for which the electronic structure can be understood as emerging from the valence electrons of the metal atoms. The interactions between these emergent superatomic states can therefore be hypothesised to lead to the observed electronic transport properties.

Here, we use Density Functional Theory (DFT) to explore the origins of electronic transport within these clusters. We employ Bader charge analysis, and study the density of states of the crystalline materials in order to describe the connection between cluster assembly structures and their electronic properties.

Then, inspired by the recent success of Campaioli and Cole in the application of the Quantum Master Equation (QME) to amorphous polymers[2], we propose an extension of our methods to an effective Hamiltonian model incorporating parameters obtained via DFT to capture the charge carrier dynamics of the system.

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P1.111 HierGO: a modular tiling approach to capturing the complexity of graphene oxide

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Graphene oxide (GO) is a complex family of few-layer materials that is growing in interest due to the versatility in its applications, from biosensors and photovoltaics, through to water filtration [1-3]. In such applications, the development and adoption of GO is informed by its structure/property relationships, which are able to be explored via structural models of GO.

Experimental efforts alone can only recover the ensemble average of GO stack structural properties, such as the C:O ratio, while properties of the individual sheets may differ. Individual sheets can vary in chemical composition, atomic arrangement and chemical bonding, and have been shown to feature heterogeneous distributions of topological defects and holes. Prior modelling efforts have mainly adopted the comparatively simple Lerf-Klinowski (LK) model [4,5] which assumes the GO sheet as an intact graphene lattice with a homogeneous distribution of hydroxyl and epoxy groups on both sides.

Here, an automated process of generating highly complex GO models via a modular tiling approach is introduced: the HierGO suite of code. With HierGO, a user is able generate complex, simulation-ready GO sheet structures to a high degree of control. As a showcase, two distinct GO stacks are modelled, comprising unique individual sheets that feature topological defects, holes and oxygen content that are varied in both concentration and distribution. Molecular dynamics simulations of these GO stacks in water reveal emergent properties such as spatially dependent inter-layer spacing, which could not be captured with the overly-simplistic LK GO stack.

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P1.113 Machine Learning for Exciton Diffusion Rates of Pentacene Dimers

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Exciton diffusion rates are a crucial determinant of the efficiency of organic photovoltaic devices. In turn, exciton diffusion rates depend upon excitonic coupling, a quantum mechanical quantity which measures how easily an exciton can pass between molecules in a dimer. Unfortunately, calculation of excitonic coupling via first-principles calculations requires considerable computational cost. These costs multiply when a large number of unique dimer pairs must be considered. In order to overcome this problem, we developed a machine learning (ML) framework for predicting exciton coupling. Our ML framework was constructed using a combination of Gaussian process regression, principal component analysis, support vector machines, and convex optimisation. Importantly, our framework can be adequately trained using a small dataset of less than 100 training data points, allowing for accurate and fact predictions of excitonic coupling without resort to large numbers of heavy first-principles calculations.

P1.114 $Sm_{(1-x)}Hf_xN$, Cation-substitution doping of rare-earth nitrides

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The continuously tuneable magnetic properties of the rare-earth nitrides (REN) offer unique spintronics opportunities for cryogenic data storage [1] and quantum-computing qubits [2]. Realising that promise demands that the conductivity is tuned to the specific devices. The structural disruption of the common nitrogen-vacancy doping [3,4] then motivates the search reported here for an alternate method of carrier concentration control.

Here we report an investigation of Hf as a substitutional donor dopant in SmN thin films. Hf is chemically similar to the rare-earths, however with a propensity for a tetravalent configuration rather than trivalent. We expect each Hf ion will substitute a Sm ion and contribute one electron to the conduction band. We discuss the implications of the Hf doping on the band structure of SmN via electrical transport and optical spectroscopy. The experimental studies are supported by, and aid in the interpretation of, first principle DFT based calculations. The results show Hf indeed dopes the system with electrons while being significantly less disruptive than nitrogen vacancy doping. Furthermore, the contrast between vacancy and Hf doping reveals a more controlled manner in which to access a heavy fermion transport channel in SmN, opening the door for a range of studies of significant fundamental interest [5,6]. This study represents a leap forward in the growth of rare-earth nitride thin films with tuneable electronic properties ideal for a host of applications.

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P1.115 Development and implementation of a multi-spectroscopic platform for the identification and biochemical characterization of cellular differences found in phytoplankton communities

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Phytoplankton communities are rapidly changing in response to ecological and environmental factors [1-3]. As a result, the identification and characterisation of cells can be used as valuable indicators in environmental water monitoring. Traditionally, statistically robust studies on combined spectroscopic data pertaining to taxonomy and growth phase cellular characteristics have been poorly studied. Herein, the taxonomic and growth phase cellular identification and characterization of three species of phytoplankton (Tetraselmis suecica, Chaetoceros muelleri and Cryptomonas sp.) was investigated using confocal NIR Raman microscopy and concurrent excitation-emission matrix (EEM) fluorescence spectroscopy

The data was analysed using two multivariate data-reduction methods: principal component analysis (PCA) and parallel factor analysis (PARAFAC) for the two-way Raman and three-way fluorescence data respectively. Subsequentially, Partial Least Squares Discriminant Analysis (PLS-DA) and Artificial Neural Networks (ANNs) were used to classify the respective Raman and fluorescence datasets. Our results demonstrate high cross-validation and prediction accuracy for different growth phases and taxonomic groups using both techniques.

To evaluate the performance of the current methodology towards complex environmental samples, Raman and EEM measurements were taken of different phytoplankton assemblages present in seawater samples acquired from Tasman Bay in the South Island of New Zealand. Characteristic shifts in pigment bands were observed for morphologically similar cells in the Raman spectra whilst the EEM data showed different landscapes and relative patterns of fluorophore specific components across differing sample locations and depths. Findings of the current study illustrate potential for future developments of combined Raman and fluorescence-based systems for use in remote water sensing.

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P1.116 Magnetic study of CoMoO4: observation of a spin flop transition

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The XMoO4 metal-molybdates, where X is a divalent metal ion, are being extensively studied for applications that include supercapacitors, lasers, and catalysts [1]. Some of these metal-molybdates also have piezochromic properties, changing colour with increasing pressure due to a phase transition from beta to alpha phases. CoMoO4 demonstrates this piezochromic behaviour around room temperature, giving it promising applications in optical shock sensing [2]. Previous reports on CoMoO4 have explored its structural, optical, and vibrational properties, but little is known about its magnetic properties except for the existence of antiferromagnetism in the alpha phase at low temperature [3].

In this report, we present the results from structural, vibrational, and magnetic studies on CoMoO4 in both alpha and beta phases. Powders of both phases were made using conventional solid-state synthesis methods. Beta-phase thin films were successfully made using RF sputtering and post annealing. Raman studies were used to investigate both phases and their relative phase fractions. Magnetic measurements confirmed the presence of low temperature antiferromagnetism and provided the first report of spin flop behaviour in CoMoO4.

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P1.117 Properties of Sn- and Si-Doped Gallium Oxide Thin Films Produced Using Sol-Gel Techniques

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Ga_2O_3 is an ultra-wide bandgap semiconductor with a high thermal stability and breakdown strength that is attracting considerable interest for power electronics, solar-blind UV photodetectors, and resistive switching [1,2]. While molecular beam epitaxy (MBE), pulsed laser deposition (PLD), and chemical vapour deposition (CVD) are commonly used to produce high-quality Ga_2O_3 thin films, the long growth times, low throughput, and high cost of these techniques prevents this material from reaching its full potential and widespread adoption.

In this research, the high-throughput, atmospheric-pressure, solution-based sol-gel technique was used to produce high-quality Ga_2O_3 thin films. This was done at growth rates orders of magnitudes higher than vacuum-based techniques, and at a fraction of the cost and energy demand, making it a promising method for the future mass manufacture of Ga_2O_3 material for electronic devices.

Both Sn- and Si-doped sol-gel Ga_2O_3 films were fabricated on c-plane sapphire substrates. This process was optimized to produce films of 100% visible transparency and very low surface roughness (~0.3 nm rms), comparable to MBE and PLD. The addition of dopants provided sufficient electrical conductivity for the fabrication of PtOx/Pt Schottky diodes with promising rectifying behaviour [3]. High-temperature annealing (500 °C to 1100 °C) in N_2 gas, formed β-Ga_2O_3 crystalline phases in the amorphous as-prepared films. At temperatures above 800 °C, Al from the substrate diffused into the films, shifting the x-ray diffraction (XRD) peak positions, and decreasing the lattice spacing of the crystalline phases [4]. This effect was investigated using XRD, UV-visible transmission spectroscopy, and atomic force microscopy.

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P1.118 Stimuli-responsive colloides for sustainable chemistry

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Welcome Function and Poster Session 1, Grand Hall, February 7, 2023, 5:35 PM - 7:30 PM

Abstract
We propose a stimuli-responsive, droplet-based support for catalyst immobilization that can selectively be "switched" on and off, through switchable compartmentalization of the cargo in droplets.1 2This will allow us to perform multiple chemical reactions within the same pot, without a need for additional purification steps. The ability to "switch off " catalysts will allow for better tolerance of a range of reactions, where incompatibility between intermediates, reagents, and products may arise.3 The droplets can then be reformed into the initial state, allowing recovery of the cargo and mitigating any potential side reactions. Therefore, there are two goals of our project, the first is to develop a new droplet-based platform for minimizing solvent usage in chemical manufacturing, and the second is to use droplets will aid in the development of supports for biocatalysts for synthetic reactions.

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P1.119 Multi-layer welding of dissimilar materials by utilizing Vaporizing Foil Actuator Welding process

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Welcome Function and Poster Session 1, Grand Hall, February 7, 2023, 5:35 PM - 7:30 PM

Welding process is one of the most important technology for attaching two different materials. Many types of materials were used as welding material such as steel, aluminum, magnesium, titanium, copper, etc.. Although there were many welding techniques to weld dissimilar materials, the welding between dissimilar materials has risks of welding defect because of different material properties, especially thermal material properties. Most of the welding techniques uses heat for welding, there are always has an issues about thermal defect such as heat affected zone, shrinkage, different melting point, etc.. Vaporizing Foil Actuator Welding process is one of the impact welding which uses vaporizing pressure of aluminum foil as a driving force of impact. In the VFAW process, two welding materials, which is called target sheet and flyer sheet, were collided with oblique angle by forming the metallic bonding between them. There is no external heat irradiation during the VFAW process, so the thermal defects in conventional welding is not considered in this process. Also, the vaporizing pressure can be additionally applied on the welded materials by forming the multi-layer welding structure. In this paper, various dissimilar materials such as Advanced High Strength Steel and aluminum were used for multi-layer VFAW process and the welding force and its material properties were estimated.

P1.120 Basin-Hopping Optimisation and Structure Characterisation Methods For Noble Gas Clusters In Strong Magnetic Fields

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Welcome Function and Poster Session 1, Grand Hall, February 7, 2023, 5:35 PM - 7:30 PM

We want to investigate the melting of noble gases [1] under the extreme conditions found on magnetic white dwarf stars, such conditions include strong magnetic fields and high pressures.

No current consistent theory can predict the characteristics of melting, so computer simulations are of great importance.

In order to properly investigate the melting mechanisms through simulations, a thorough understanding of the potential energy surface, PES, is needed.

Such a PES is characterised by a huge number of local energy minima separated by high energy barriers. Here, we investigate how the PES of neon clusters is influenced by strong magnetic fields using an optimisation method called basin-hopping [2], which consists of random perturbations and local minimisations.

This allows us to identify new local and global minima of neon clusters, as well as their connectivity in strong magnetic fields.

To classify and compare structures, we use a structural comparison method [3] based on common neighbour analysis, which finds the fingerprints of pairs of atoms to characterise their local environment.

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P1.121 Shelf life enhancement of agricultural products via coating of simply synthesized nanoparticles

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Welcome Function and Poster Session 1, Grand Hall, February 7, 2023, 5:35 PM - 7:30 PM

Aim: Fresh produce is the major source to increase revenue, therefore, quality management and prevention of postharvest losses are very important. Among all, fruits are the extensive and essential fountainhead of micro-nutrients and phytochemicals which are required for human well-being. When coated with some metallic nanoparticles, the shelf life of fruits can be significantly enhanced. Moreover, this research highlights the strong impact of nanotechnology on the increased shelf life of products in the agricultural industry around the globe.

Content of Presentation: Here we report the coating of biologically synthesized metallic nanoparticles over the lemons to investigate the variation in shelf time. Specifically, silver (Ag) and zinc oxide (ZnO) nanoparticles (NPs) were prepared via green synthesis using freely available neem leaves. Furthermore, the samples have been characterized using various microscopic and optical spectroscopies to study morphology as well as the operating of the optical range of nanoparticles. After coating over lemons, the weight loss percentage showed a direct relation to the concentration of ZnO while an inverse relation for the case of Ag. This is because the ZnO nanoparticles exhibit a strong pathogenic effect. Furthermore, the weight loss under ZnO nanoparticles is much lower at 100ppm and 1000 ppm as compared to Ag nanoparticles. So, it is concluded that the Shelf time enhancement is only possible due to the 'unique' anti-microbial properties of silver [1, 2] and ZnO nanoparticles [3-6].

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P1.121 Materials Intermixing and the Dipole Formation at the TQ1/Conjugated Polymer P(NDI3N-T-Br) Interface

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Welcome Function and Poster Session 1, Grand Hall, February 7, 2023, 5:35 PM - 7:30 PM

Organic photovoltaics (OPVs) are fabricated using varied types of organic or polymer materials. Generally, they are widely available and require low-energy fabrication techniques, which explains why they have gained considerable attention over the years. OPVs still display numerous advantages over their inorganic equivalents. They include low-cost organic material requirements, affordable scalable range of fabrication techniques, versatile design and portability. Interfacial studies of different layers in polymer have played an important role on exaction separation and charge transport. In this project, P(NDI3N-T-Br) polymer used as n-type layer in organic based solar cell with different thickness of the TQ1 polymer on the top of P(NDI3N-T-Br) on indium tin oxide (ITO) substrate. The film thickness was investigated using Neutral impact collision ion spectroscopy (NICISS) technique with low energy ion scattering that utilize the ion at the surface to detect the elements, this technique was used to determine the thickness of the active layer (TQ1) to achieve a closed thin layer with few nanometers (nm). Also, to determine how deep the TQ1 penetrates the polymer P(NDI3N-T-Br). Our investigation shows that upon deposition of the TQ1, a strong dipole is formed at the interface between the active layer and the P(NDI3N-T-Br). The strength of the dipole increases with increasing thickness of the TQ1 layer. It has been known that the interface dipole has important consequences for energy level alignment in organic interfaces and various aspects of OPV performance, including charge separation and recombination rates, and the open circuit voltage. This work also established a clear understanding of the work function, energy levels measurements of active interface layer and how the energy levels of all materials depend on the thickness of TQ1. The work function of the P(NDI3N-T-Br) was found to be independent of the thickness of TQ1. Moreover, we attribute the difference in performance to the ratio of the Bromine in the P(NDI3N-T-Br) as determined by XPS. The physical and electronic model of the interface region was obtained from Ultraviolet Photoelectron spectroscopy (UPS) and Inverse Photo Emission Spectroscopy (IPES).

Poster Session 2

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P2.001 SmartBioplastics – Extending food shelf-life and reducing environmental impact through bio-based active packaging materials

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Poster Session 2 + Tech Tasters Pitch Sessions, February 8, 2023, 5:35 PM - 7:30 PM

Contamination of edible goods with pathogens and spoilage microbes is a significant issue in New Zealand and globally, resulting in shortened shelf-life, increased health risks, and food wastage [1,2]. Efforts to reduce this impact are essential to improving global food supplies and offer significant benefits to New Zealand's export industries. One approach is using smart and active packaging materials that suppress microbial growth on packaged goods [3,4]. While commercial solutions exist, they currently rely on synthetic plastics derived from fossil resources and do not naturally degrade upon disposal.

Recently, the MBIE Endeavour SmartBioplastics project was initiated, bringing together a global team with biotechnology, polymer, and material science expertise. This collaboration will create fully bio-based, compostable, and/or edible active packaging materials which protect food and extend its shelf life.

Our objective is to develop functionalised bioparticles that suppress the growth of food spoilage microorganisms and foodborne pathogens. These bioparticles will be processed into formulations to be deposited onto bioplastic films using coating technologies suitable for industrial-scale manufacturing. The model system we will focus on consists of active packaging for fresh meat products, targeting the widespread bacteria Clostridium (causing food spoilage) and Campylobacter (causing foodborne diseases). This presentation will introduce the fundamental concepts, our scientific hypotheses, the planned experimental approach, and some preliminary results obtained thus far.

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P2.002 Watching Ternary Oxides with Dual Eyes:in-situ Two-Colour XES Studies of Chemical Transformations & Electronic Structure in Ferric Pseudobrookite (Fe2TiO5) Photoanodes

Mr Devi Prasad Adiyeri Saseendran[1], Dr Sergey Peredkov[2,3], Dr Carlos Triana[1], Dr Daniel Abbott[4], Prof. Dr Victor Mougel[4], Prof. Dr Serena DeBeer[2], Prof. Dr Greta Ricarda Patzke[1]

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Poster Session 2 + Tech Tasters Pitch Sessions, February 8, 2023, 5:35 PM - 7:30 PM

The design of highly efficient, robust, and green water oxidizing catalysts is one of the most critical challenges in sustainable energy research. Due to the global climate change crisis and energy demand, solar assisted photo-electrocatalytic (PEC) water splitting has emerged as a promising approach towards producing clean chemical fuels and storable energy resources. An ideal photo-electrode material encompass suitable energy bandgap for efficient sunlight absorption, good electrical conductivity, chemical stability, and non-toxicity. Among the investigated photoanode materials, α-Fe2O3 had gained considerable interest in the field due to its suitable bandgap (1.9-2.2 eV) and earth abundance. Doping α-Fe2O3 with tetravalent dopants such as Ti4+, Zr4+ had been found to increase its carrier conductivity, thereby improving the PEC performance. In this regard, ternary oxide materials have emerged as potential candidates for photoanode materials, as they provide diverse strategies for tuning the composition and electronic structure of photoanode materials compared to their binary counterparts. Among these, the ferric pseudobrookite: Fe2TiO5 has received significant attention owing to its high thermodynamic phase stability, aqueous stability in a wide pH range, and suitable bandgap (1.9- 2.1 eV) for efficient solar light absorption. Herein we report Fe2TiO5 inverse opals photoanodes which has shown improved performance and photocurrent density under solar light irradiation. We demonstrate the use of two-colour X-ray Emission Spectroscopy (XES) in identifying the catalytic intermediates and electronic structure changes involved in solar water oxidation catalyzed by Fe2TiO5 photoanodes, via Fe-Ti two-colour VtC-XES experiments under operational PEC conditions. In-situ XES studies indicated that the Ti sites acts as oxo-coordination site whereas the Fe site behaves as a redox regulator. Further post-catalytic XAS and XPS investigations also confirmed the change in local coordination at the Ti center, confirming its active role in driving the O-O bond formation.

P2.003 Use of solar-powered wearable UV monitoring clothing and public health displays in school-based skin cancer prevention programmes

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Excessive UV exposure in childhood and adolescence is known to significantly increase melanoma risk in adulthood, while lifetime patterns of sun exposure and protection are known to be strongly influenced by knowledge, attitudes, and behaviours acquired while at school [1]. This makes school-based SunSmart education programmes a significant primary skin cancer prevention opportunity [1].

We have increased the efficacy of existing school-based SunSmart programmes by including the use of real-time UV data acquired using solar-powered wearable UV dosimeters and clothing. These are worn by students as they carry out their own scientific investigations into the nature of solar UV radiation. Activities include investigating the protection provided by hats, clothing, shade, sunglasses, and sunscreen using data measured and analyzed by the students themselves. Solar-powered public health displays are also set up around the school, both during and for several weeks after the intervention, to continuously display UV levels and deliver SunSmart reminder messages to ensure that the lessons learnt are reinforced and retained [2].

By participating in a systematic investigation in their own school environment, students personally learn about the nature and risks of UV radiation rather than just being told about it. Levels of engagement are significantly higher when students directly learn about the effectiveness of SunSmart behaviours compared to non-experiential programmes [1]. As a result, the efficacy of school-based SunSmart education programmes has been significantly improved by the use of a range of real-time UV measures including wearable UV dosimeters, UV monitoring clothing, and solar-powered electronic UV displays.

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P2.004 Targeting Extracellular Vesicles from Breath as a Diagnostic Tool

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Research in the area of extracellular vesicles (EV) have exploded due to their novel biomedical applications, such as disease diagnosis or drug delivery. Extracellular vesicles are defined as nano-sized particles that have a lipid bilayer. They are released by all cells and are found in most body fluids such as blood, plasma, serum and breast milk; even exhaled breath. Their composition and physical properties are unique to the cell of origin. In particular, their biogenesis imparts "cargo" molecules such as transmembrane proteins that show much potential to serve as disease biomarkers. Therefore, EVs can be used to determine whether a cell is healthy or diseased. The first report of isolation and full characterisation of breath-derived EVs was published by our research group[1]. Based on the earlier findings, this project investigates the use of extracellular vesicles as a non-invasive route to detect lung cancer. Gold substrates were modified using self-assembled monolayers and aptamers for the detection of CD proteins (common target proteins found on EV membranes). Electrochemical impedance spectroscopy measurements showed an increase in resistance upon EV capture, complemented by results from surface plasmon resonance. Choice of aptamer, alkanethiol, period of immobilisation and modification route, emerged as significant factors that can influence the ease of fabrication and platform performance. Successful adaptation could provide a cheap, rapid and non-invasive platform for diagnosis of lung cancer and other related problems[2].

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P2.005 Opportunities for 3D-printed Nanomachines in Biological Studies with Optical Tweezers

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Improvements in micro-nano manipulation and visualisation techniques have brought about exciting and disruptive changes in biological studies over the last few decades. This has enabled the rise of sub-cellular and single-molecule studies, which have been performed using relatively well-established tools such as magnetic [1] and optical tweezers [2]. These established tools can be augmented by making use of advances in micro-manufacturing- particularly nanoscale 3D printing [3]. Printing on the nanoscale has allowed researchers to create complex, interestingly structured auxiliary tools to use as end-effectors [4], rather than being reliant on simple microbeads. As optical and magnetic tweezers are dependent on the resolution of changes in an electromagnetic field to manipulate objects, the use of auxiliary tools can be helpful to produce movement that is otherwise difficult to achieve- including out-of-plane rotation [5] and even force amplification [6]. Additionally, optical tweezers can damage samples due to exposure to intense laser radiation [7], and 3D printed nanomachines can be used to mitigate this by distancing optical traps from the target.

This presentation covers our work in developing and investigating the use of optical nanomachines for biological studies. This work centres around our use of optically actuated microlevers to stretch DNA [8] and amplify optical forces [6]. Additionally, we will discuss our recent investigations into encoding functionality in optical nanomachines through parameter choices during the printing process and possible uses for such tools in biological research.

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P2.006 Electro-reduction of Ilmenite in Alkaline Media

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Ilmenite (FeTiO3) is an abundant mineral and ferrotitanium alloys are among the earliest known hydrogen storage materials. FeTi alloys are also key materials in the metal industry for the deoxidation of steel and iron, welding rod flux and magnetic materials.1 Iron and titanium co-exist in ilmenite with a known world total resource of ~2X1012 Kg.2 However, the two metals are currently separately extracted in the industry by carbothermic (Fe) and magnesiothermic (Ti) reduction methods, with the former process emitting about 5x1011 Kg CO2 per year.

There is substantial global interest in alternative metallurgical processes which can reduce the greenhouse gas footprint of the metal industry. One such approach is the electro-winning using electricity generated from renewable sources. New Zealand is uniquely placed to develop such technology as its electricity generation system comprises >85% renewable sources. Here, we report initial investigative work into the electro-reduction of ilmenite (FeTiO3) through electrolytic decomposition in an aqueous alkaline electrolyte. It has been shown that electro-reduction of alkaline slurries of iron oxide powder can proceed similar to the Fray-Farthing-Chen (FFC) mechanism.3 In this work, slurries of ilmenite powder were formed through suspension in concentrated aqueous sodium hydroxide solution. It was observed that applying a constant current at temperatures above 100 oC led to the evolution of oxygen at the inert platinised titanium anode. At the same time, Fe metal alloy was deposited at the cathode containing ~3.9% Ti. In order to evaluate the industrial feasibility of this process, we have experimentally measured the current efficiency and cell voltage in an optimised cell configuration and used these values to calculate the corresponding process energy cost. We have also studied the influence of cell parameters on the morphology of the resulting iron deposits, and characterised the contaminants present within these electro-deposited films.

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P2.008 Elucidating the Conducting Mechanism in Reduced-Graphene Oxide Porous Film as Pressure Sensor

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Using a porous film made from reduced-graphene-oxide (rGO) embedded in an elastomer as a sensitive pressure sensor has been demonstrated [1], where all the electrodes are on the same side. The increase in resistance with pressure of the sensor exhibits two distinct linear regions, up to ~10 kPa being a steeper gradient that over ~10 kPa. This could indicate the presence of two conduction mechanisms [2], which were investigated by measuring the variation in resistance with temperature at high (28.5 kPa) and low (0 kPa) pressure. The variation with temperature indicates that the low-pressure conduction mechanism is dominated by Schottky emission, and at high pressure by a hopping mechanism becomes significant. This can be explained by the deformation of the sensor under compressive load, with low pressures primarily causing an orthogonal tensile strain and the corresponding increase of work function (and therefore resistance) [3]. In the high-pressure region (corresponding to over 20% compressive strain) the porous structure of the foam begins to collapse, resulting in increased probability of hopping between traps occurring. This hopping distance will continue to reduce with increasing pressure, leading to a reduction in resistance. The onset of this conduction mechanism is overlaid onto the conduction due to Schottky emission, leading to the shallower gradient of resistance against above ~10 kPa.

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P2.010 Classification Model of Paper used in New Zealand One Penny Stamps (1936 to 1953) utilizing Near Infrared Hyperspectral Imaging Spectroscopy

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This project demonstrates how spectroscopy and chemometrics could be used by stamp collectors to identify stamps. It focuses on stamps produced from 1936 to 1953 with varying composition due to supply chain problems caused by World War 2. From prior work the most promising technique to differentiate the stamps is Near Infrared (NIR) hyperspectral imaging spectroscopy of the paper, with Partial Least Squares Discriminant Analysis (PLS-DA) being applied. The PLS-DA model also revealed, an anomalous sample. Excluding this sample, the other data was used to construct a prediction model, that indicated that this sample was misclassified. Independent of this knowledge, a review of philatelic sources concluded that a range of stamps produced during 1939 could have been misclassified, as it is not clear what type of paper was used.

To resolve this conundrum, a more accurate PLS-DA model was constructed and validated using NIR hyperspectral imaging spectroscopy of stamps of known type. This model can now be used on stamps produced in the era where the paper type is unknown and classify them. Without this work normal philatelic ways of examining stamps struggle to differentiate stamps produced between 1936 to 1953, let alone come up with a conclusive way to classify stamps produced during 1936. This project shows how science can be used in a novel way within society to help solve problems.

P2.011 Towards a circular silicone economy in Aotearoa

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Aotearoa/New Zealand's "clean, green", "100% pure" visage is a fundamental part of its national identity, and a key promotional tool for the tourism industry. The country's management strategies for complex wastes detract from this image, as many are landfilled or exported. One such complex waste stream is that of silicones, which have high thermal and chemical tolerances, and are generally biocompatible, making them critical materials in medical technologies, consumer goods, industrial applications, and construction.[1] Further, their production from primarily non-fossil-fuel sources makes them a potentially more environmentally friendly alternative to organic plastics. While some un-crosslinked silicones readily biodegrade in the environment,[2] crosslinked products like silicone rubbers pose a challenge for waste management.

Silicone production involves high energy processes and hazardous reagents on large scales.[3] Despite the associated environmental concerns, the material's relative affordability has limited the advancement of recycling technology in this area. Some mechanical 'downcycling' methods have emerged[4] but provide lower quality products with limited applications. Novel chemical degradation strategies[5] for siloxanes may offer a pathway towards a cyclic silicone economy that can reduce energy consumption, while offering products of equivalent quality to virgin material. An investigation into chemical and environmental degradation methods for siloxanes is underway to identify strategies that will be viable for the scale and waste profile of Aotearoa. Embracing the principles of green chemistry, and aiming to minimise steps involved, this approach is exploring several levels of degradation / regeneration to develop a model for an environmentally and economically sustainable circular silicone economy.

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P2.013 Novel Long-Term Packaging Material for Wireless Implantable Devices

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Implantable electronic devices that are designed for long-term use are generally enclosed by a hermetically sealed titanium container [1]. Although this design provides watertight protection from the bodies chemically harsh environment, it prevents the device being used with wireless applications. One solution to this limitation is to use a polymeric enclosure (or lid on a titanium enclosure).

A polymer can be injection-moulded and is transparent to electromagnetic waves. This allows for the transmission of wireless signals and/or power to an external device [2]. However, polymers still have some limitations preventing their adoption for long-term applications. Although some polymers, such as liquid crystal polymers (LCPs), have low moisture absorption rates, they are never zero, because water molecules can travel from the body through the polymer, increasing the humidity and affecting the operation of the implanted electronics [3].

The aim of this research is to increase the lifetime and robustness of a polymer-based packaging technology that could ultimately provide an increased usable lifetime for an implanted sensor. This research project investigates the usable lifetime of electronics encapsulated in a sealed, LCP housing. Based on earlier testing using acrylic lids on titanium housings with an epoxy sealing method, experimental testing will involve monitoring moisture ingress into a fully LCP polymer package using an internal, wireless, relative humidity sensor.

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P2.014 Three-dimensional percolating networks of nanoparticles

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Percolating networks of nanoparticles (PNNs) have been proposed as a key component in neuromorphic (brain-like) computing systems [1]. The PNNs are composed of conducting particles that are randomly deposited on a planar insulating surface and which coalesce into groups separated by tunnel gaps. Within the gaps, atomic filaments can form/rupture under an applied voltage. This creates a dynamic network structure which can be represented by a planar graph (nodes = groups, edges = tunnels/filaments) [2]. To date most experimental devices are two dimensional (2D): here we report on simulations of the properties of 3D networks that can by created by co-deposition of nanoparticles and an insulating matrix.

We study the effects of system size on square 2D systems and cubic 3D systems. We compare instances of square and cubic systems for which a similar total number of particles are required to reach comparable proximity to the percolation threshold. Our results indicate that while the degree distributions for 2D and 3D are quite similar, the number of groups in the networks is much higher in 3D (by a factor 3.8). Furthermore, using a previously reported method for determining the dominant current paths through the simulated networks [3], we show that relatively more such paths are apparent in 3D systems, suggesting that a higher level of complexity may be able to be exploited for neuromorphic computing. We conclude that here is sufficient evidence to warrant experimental studies of 3D composites.

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P2.015 A Novel Approach Towards Plasma Assisted Landing of Biomolecular Structures

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In the wake of the pandemic, we continue to find ourselves in a world controlled by long and arduous disinfection protocols. Traditional antimicrobial cleaning techniques typically involve dangerous, volatile chemicals, or extreme heat which can severely damage delicate materials. We propose to take a novel approach to addressing this issue, utilising an open atmospheric plasma jet to create surface coatings which are highly functional, controlling the properties of the plasma to manipulate features of the surface coating. This proposed approach will provide a bespoke and tailored approach to cleaner, smarter, and safer surface coatings.

Utilising the plasma jet species, we will demonstrate the behaviour of biomolecules when exposed to the plasma jet. We propose a novel solution utilising an Atmospheric Radiofrequency-Pulsed Plasma Jet to develop functional, tailored antimicrobial surfaces. Our bespoke plasma system produces a low temperature plasma under atmospheric conditions. The custom plasma jet set up, introduces a radio-frequency pulsed plasma jet where we explore the potential of the biomolecules to adhere to the surface and the ability to control morphological structures of the deposited material. Fine tuning the plasma properties grants us control over the orientation of biomolecules, and other particular properties of the surface coating such as density and porosity, resulting in a fully customisable coating.

P2.016 Assembling At The Interface: Introducing Automation Into Colloidal Swarm Dynamics With Optical Tweezers

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Swarm and collective behaviour in robotics has long taken inspiration from the natural world at a range of size scales: macro-scale, such as, birds flocking, fish schooling, colonies of ants and bees searching for food; micro-scale, such as bacteria migrating and quorum sensing. Micro-scale robotic swarms often consist of simple colloidal agents which require external energy (acoustic forces, magnetic fields, chemical gradients, light gradients and optical force) to manipulate self-organizing abilities producing coordinated swarm and collective behaviour. The use of optical tweezers (OT) on colloidal particles at the air-liquid interface provide an interesting self-organizing dynamic where the trapped particle scatters and propagates the laser, expanding optical potential, attracting particles from outside of the lasers focus [1]. First, the assembly forms a kinetic state referred to as concentric circular (CC)-like assemblies, the assembly then reorders into a thermodynamically stable structure known as hexagonal close packed (HCP)-like assembly through ejecting particles in a pistol-like fashion. Research groups have tuned various parameters in an effort to form greater control over these swarms such as laser power, optical force absorption [1], surface charge and surface tension [2]. Automation in the OT space has become more viable since the development of holographic optical tweezers (HOT) and has been implemented in the manipulation of cells, measuring interactions between pairs of colloidal particles and more. Our project uses high power OT traps to form these assemblies then autonomously grow, manipulate and control the swarms dynamics through HOT and Red Tweezers software with a custom plugin [3].

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P2.017 Packing microstructures and thermal properties of compressed emulsions: effect of droplet size

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In preparing thermodynamically metastable emulsions, the droplets tend to coalesce. Consequently, it is difficult to investigate the properties of a monodisperse compressed emulsion experimentally or by simulations. At a specified volume fraction, the properties of emulsions vary with the droplet size but the relevant studies are very limited. The dissipative particle dynamics simulations are adopted to explore the highly concentrated emulsion of monodisperse droplets.[1] Prior knowledge of the microstructure and inter-droplet interaction is not required. The critical packing associated with the onset of the jammed structure can be identified from the growth of the projected area and perimeter of droplets with the volume fraction (ϕ), $\phi c \simeq 0.65$. The mean coordination number (Z) from the radial distribution function rises with increasing the volume fraction and can be described by the scaling relation $(Z-Zc) \sim (\phi-\phi c)^{0.82}$ with $Zc \simeq 6.3$. The effects of the volume fraction, droplet diameter (D), and interfacial tension (σ) on the internal energy (U) and heat capacity (Cv) are studied systematically. Both U and Cv are found to grow as ϕ and σ are increased but D is decreased. According to dimensional analysis, all the data points can be well represented by the scaling relations $(Cv-Cv,c) \sim (\phi-\phi c)^{1/3}(\sigma/D)$ and $(U-Uc) \sim (\phi-\phi c)^{1/3}(\sigma/D)$.

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P2.018 Cell scaffolds formed from protein nanofibrils

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Amyloid fibrils are historically associated with human diseases. However, they are also a source of new materials. Their characteristic structure of cross-beta sheets contributes to their potential to be stable and mechanically robust building blocks[1], and they have shown promise in various applications such as biosensor[2], small molecule carrier[3,4], and scaffolds[5]. This study focuses on hemoglobin nanofibrils, which we use to generate cell scaffolds with improved biocompatibility for tissue engineering. Nanofibrils were formed via pH and temperature treatment of bovine blood-extracted hemoglobin resulting in the re-arrangement of the globular proteins into nanofibrillar structures. Taking advantage of the stability of these nanofibrils, they can be integrated with polycaprolactone polymers via electrospinning, which enables their transformation from a liquid state to solid cell scaffolds.

In this project, transmission electron microscopy and the selective dye Thioflavin T were used to confirm the presence of amyloid fibrils. Cell viability tests (e.g., PrestoBlue assay and Live/Dead cytotoxicity kit) and scanning electron microscopy were carried out to further prove the feasibility of using these electrospun mats as cell scaffolds. Overall, this work exhibits the possibility of using protein nanofibrils as cell scaffolds and encourages further exploration of using industry low-value products, such as bovine blood, as an economical fibril source to create functional biomaterials.

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P2.019 Oral toxicokinetics and fates of differently manufactured food additive silicon dioxide in rats

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Food additive silicon dioxide (SiO2) is widely used as anti-caking agents in the food industry. SiO2 can be classified as pyrogenic (fumed) and precipitated SiO2 depending on manufacturing methods. Along with rapid development of nanotechnology, it is probable that SiO2 particles are also produced as nanoparticles (NPs). However, the presence of NPs in two differently manufactured SiO2 and their physicochemical characterization have not been well determined, which can affect toxicokinetic behaviors and toxicity. In this study, fumed and precipitated food additive SiO2 particles were characterized in terms of particle size distribution, surface area, and zeta potential values, and solubility. Oral absorption, tissue distribution, and excretion kinetics of both SiO2 particles were evaluated in rats. The results demonstrate that the constituent particle sizes of SiO2 particles were less than 100 nm, but present as aggregates. Their solubilities in biological fluids and oral toxicokinetics were affected by manufactured type. These findings will provide basic information about safety aspect of food additive SiO2 NPs.

P2.020 Nano and micro-interdigitated electrodes for enhanced electrochemical biosensing

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Electrochemical biosensors (EBs) have great potential for point-of-care (POC) diagnosis and are suitable for health and environment monitoring due to their low cost, rapid testing, simple operation, and miniaturization[1]. However, technical and commercial challenges remain, including sensitivity, stability and specificity[2]. Among various EBs, an interdigitated array of electrodes (IDEs) is a promising electrode geometry that has attracted interest for its high sensitivity, as it enables rapid mass transport between the electrodes and amplifies the redox signals due to their close proximity and small dimensions involved[3].

Reducing the width and gap between the adjacent electrodes of an IDEs substantially increases redox current, allowing lower amounts of analyte[4] But the advantages and disadvantages of further reducing IDE dimensions (from micro to nanoscale) on a sensor's performance are not well characterized in the literature, the understanding of which would significantly advance EB design and performance. Here, we have designed and developed micro-IDEs using photolithography and nano-IDEs with e-beam lithography. They are characterized by their electrochemical responses with the redox cycling technique using the ferro/ferricyanide model system. The current response is linear with concentration with improved redox cycling efficiency (sensitivity) in the nanoscale. As a proof of concept, we also demonstrated the detection of streptavidin with biotin-modified IDEs. The ability to reliably transport and sense in microliter volumes of analyte solution with high sensitivity is a remarkable advantage for analytical purposes.

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P2.021 Single Electrode-to-Single Neuron Interface via Specific Biomolecular Association

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Of great importance is single cell-to-single electrode interface in terms of fundamental addressing live cells by electrochemical methods. That is a representative example of neuro-electric bilateral interface. It is crucial for this goal to constitute highly specific synapses onto electrodes maintaining a stable and long-lasting interface. One of possible approaches is to place ligands on the electrode surface that would be bound through protein-protein interaction to specific parts of neuronal cells. We functionalize the surfaces of micropatterned ultramicoelectrode with genetically engineered neuroligin-1 protein to demonstrate the formation of nascent presynaptic bouton upon binding to neurexin-1β on the presynaptic membrane of neurons. The resulting synaptically connected electrode let itself specifically bound to presynaptic proteins, triggering exocytosis just like that of native synapses. Importantly, neuroligin-1 induced synapse-electrode interface exhibits type-specificity and structural robustness. We envision the use of synaptic adhesion proteins in modified neural electrodes may lead to new approaches in the interfacing of neural circuity and electronics.

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P2.022 Investigating Reversible Assemblies of Janus Particles

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Colloidal self-assembly is a powerful strategy for developing technologies where nano- or micro-scale particles self-organise into structures with emergent properties [1, 2]. One particular type of particles of interest is asymmetric colloids known as Janus particles. The anisotropic nature of these particles introduces directionality in particle-particle interactions [3] and for amphiphilic particles these interactions are dominated by the hydrophobic attraction [4]. However, further study is needed to better understand the dynamics of these interactions, and how they are influenced when Janus particles are suspended in a microfluidic channel with continuous flow.

In the present work, we study the dynamics and assembly of Janus particles inside a sheath-flow microfluidic channel. We have trialled two strategies for fabrication of amphiphilic Janus particles that are visible with optical microscopy (~10 µm). Firstly, gold has been deposited on polystyrene spheres prior to functionalisation with thiol groups. Secondly, hexamethyldisiloxane (HMDSO) has been deposited on silicon spheres using atmospheric plasma jet printing. In both cases, shadowing of one hemisphere from the directional deposition creates the Janus asymmetry. We characterise particle-particle interactions by their orientation as a function of position through the microfluidic channel, and our latest results and analysis of these experiments will be presented.

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P2.023 Reconfigurable droplets from light-switchable supramolecular building blocks

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Using Nature as inspiration, where living systems operate in a constant cycle of reconfiguration, reconfigurable droplet systems are researched as dynamically reconfigurable systems that change and perform chemical reactions in a sustainable way.

However, control of reconfigurable complex systems faces limitations by the methods of control, in that multiple types of stimuli change the properties of the system by introducing or influencing different aspects of the chemical environment (e.g. when pH of a solution is used as a trigger). That can lead to potentially unwanted interactions with the species present in the reaction mixture. Light is a clean option for a stimulus as it does not add any additional components and is easily introduced to a system.

This research concerns the design, synthesis, characterisation and utilisation of a reconfigurable droplet system based on amphiphilic compounds that isomerise in light and change their polarity, and thus solubility, as a result. We investigate two promising photochrome species, spiropyrans[1,2] and DASAs[3] (Donor-Acceptor Stenhouse Adducts) with the aim of assembling droplets that will behave as nanoreactors for a complex system of reactions, where the light will act as a functional switch to activate the nanoreactors.

We will present our initial results on the project and discuss future directions and application opportunities of such systems.

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P2.024 Understanding the Forever Chemical Problem in Aotearoa NZ

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Per- and polyfluoroalkyl substances (PFAS) are a class of man-made chemicals (>4000) with a partially or fully fluorinated carbon chain. Developed in 1940s by 3M, these compounds have unique properties to repel oil, water and grease and have remarkable chemical, biological and thermal stability due to strong C-F bond. Thus, they have widespread use in a myriad of consumer and industrial products namely, waterproof clothing, non-stick cookware, food packaging, personal care products, electronics, stain-repellent carpets and firefighting foams. Due to their immense usage and persistence, these chemicals are ubiquitous on our planet – in water, soil, plants, terrestrial and aquatic food chain, blood and even in the remotest areas of Mt Everest[1] and Arctic.[2] Notably known as “forever chemicals”, PFAS are highly persistent, bioaccumulative and toxic (PBT) and very mobile.[3] Owing to their health and environmental concerns, and analytical improvements, there has been increased attention towards regulating, remediating, phasing-out, and substituting to these Chemicals of High Concern (CoHC). Though PFAS are not manufactured in NZ, recent studies have found their occurrence in NZ common dolphins,[4] urban waters[5] and rain water.[6] This presentation aims to highlight results from NZ specific studies, focusing on PFAS contaminated sites and affected iwi due to their historical use at defense and aviation sites for firefighting training. Other sectors where PFAS are being imported and used in NZ, will also be discussed. The current state of knowledge on emergence, distribution, remediation, and replacement in Aotearoa NZ will help raise awareness for this next global public health emergency.

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P2.025 Fabrication of Gas Sensors Using Plasma Jets

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Plasma-enhanced chemical vapour deposition (PECVD) is an established fabrication method for the deposition of thin films and nanocomposite coatings.[1, 2] Recent efforts have seen the development of atmospheric pressure plasmas, which eliminate the need for vacuum equipment and provide pathways to 'solvent-free' continuous processing which is more efficient for industrial applications.[3, 4]

This poster presents novel work using an aerosol-assisted atmospheric pressure plasma jet printer (AA-APPJP), in which aerosolized feedstock materials are injected into a plasma jet and printed on a substrate surface. The aerosolized precursor is exposed to the highly active plasma region, undergoing a number of chemical and physical transformations during deposition.[5]

Early work focused on the fabrication of tungsten trioxide (WO_3) films utilising a colloidal hydrated WO_3 feedstock stabilised in oxalic acid. Microscopic and spectroscopic based characterization revealed complex spherical microstructures, assumed to composed of plasma-polymerized oxalic acid and WO_3 platelets. The crystal phase of plasma deposited WO_3 could be controlled by altering the plasma conditions under which the films were deposited. These films have many potential applications including gas sensing, window glazing and photocatalysis.[6]

Current work moves towards the use of AA-APPJP for the 1-step fabrication of complex metal oxide solid solutions (E.g., WxMoyOz), while maintaining the unique microstructures observed previously.

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P2.026 Piezo-photocatalytic and Photocatalytic traits of monoclinic BiVO4 with Anti-bacterial Property

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Piezo-photocatalysis, a process that combines the piezoelectric and photoresponsive behaviour of materials, is considered a promising strategy for water treatment. Here, we look at the photocatalytic, piezocatalytic, and piezo-photocatalytic responses of bismuth vanadate (BiVO4) nanorods when excited by chosen visible light and ultrasonic frequencies (35 kHz). The creation of BiVO4 nanorods was accomplished using a simple hydrothermal method. The prepared samples were then calcined at three different temperatures—300 °C, 500 °C, and 700 °C (C300, C500 and C700). They all crystallize into the monoclinic scheelite phase. BiVO4 nanorods stand out for their extended visible-near-infrared (Vis-NIR) absorbance and high Bi5+/Bi3+ and V4+/V5+ ratios, which suggest a high concentration of oxygen defects. Piezoresponse force microscopy (PFM) along with the ferroelastic measurements confirms the polarization in C300 and C500. The photo and piezo behaviour are tested with methylene blue (MB) as a standard organic pollutant. The piezocatalytic and piezo-photocatalytic processes are initiated in BiVO4 through feeding ultrasonic mechanical vibrations. Consequently, this elicits the charge polarization and separation in BiVO4 nanorods. It is found that piezo-photocatalysis is dominant for a short period, but eventually, it slows with time. This can be ascribed to sonication's fracturing effect, which further exacerbates the catalytic process due to the damage to the catalytic sites. In addition to this, the photocatalytic inactivation of Gram-positive (Staphylococcus aureus) and Gram-negative (Escherichia coli K12) bacteria was investigated under visible light irradiation using C300 and C500 samples. Within 120 min, C500 exhibited superior mortality rates compared to C300.

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P2.027 Porphyrin-like designer catalysts for electrocatalytic H2 evolution and selective CO2 reduction

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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 'brown' hydrogen made from fossil fuels in energy intensive and carbon emitting processes, so this must also be replaced by green hydrogen.

Catalysts are needed to reduce the energy of chemical processes, such as HER and CO_2RR,[2] to make them more energy and cost efficient. The CO_2RR is an energy intensive 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 both homogenous and heterogenous conditions, the latter 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 electrochemical HER and CO_2RR testing on selected complexes.

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P2.029 An upper bound visualization of design trade-offs in adsorbent materials for gas separations.

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The last 20 years have seen an explosion in the number of publications investigating porous solids for gas adsorption and separation. The abundance of materials (this work identified 1608 materials for CO_2/N_2 separation alone), makes selecting materials to use in process modelling challenging. The field lacks a unifying resource to assess new material advances against the current state of the art.

In this work, simple adsorption metrics (capacity, selectivity and heat of adsorption) are explored using a bound visualization that empirically correlates the trade-offs typically encountered when designing adsorbent materials.

Bound visualizations have been applied to a range of gas pairs involving CO_2, N_2, CH_4, H_2, Xe and Kr. We examine the leading materials to elicit the most promising design strategies for breaking traditional design trade-offs. The result is a visual tool that can be used by process engineers to select candidate materials with the best balance of properties for their process and by materials scientists to place their material discoveries in the context of the wider field.

P2.030 Determination of the impact forces applied to the polo ball during match play.

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During match play the polo ball is subjected to extreme impact forces that enable it to travel at speeds of up to 160 mph or 200 km/h. These forces are seen to affect the ball in such a way that they fail prematurely and may need to be replaced more than twelve times during a match. The balls themselves have undergone changes over the years, initially made from animal hide, laminated cane, and more recently polymer [1].

The polymer balls even with short-lived performance are an improvement on the traditional materials due to reduced cost several issues have been raise by various stakeholders in the polo community. Some players question the variability of balls (durability and performance), the pricing, and availability, with only one NZ source, despite the advanced polymer manufacturing industry [ref]. From a manufacturing perspective, the process is labour intensive and has a high rejection rate [2]. There is also the societal shift from reliance on petroleum based raw materials to consider.

This research sets out to address, firstly through understanding the dynamic mechanical properties involved during play, the performance parameters that the ball is required to meet [3].

We start with determination of the equivalent maximum force at impact required to enable the ball to be launched. The maximum force at launch will determine the intrinsic response of the ball.

Considerations are, line of action, location of impact, mass of ball, geometry of ball and contact time.

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P2.031 An impedimetric, antibody-free 25-hydroxyvitamin D3 sensor based on silver/silver oxide/carbon nanotube composite

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Vitamin D is a micronutrient crucial for the human body due to its significant role in bone metabolism. Its deficiency in the body is a worldwide health concern with major consequences on bone health. Various studies have also linked the deficiency to cardiovascular diseases, depression, infectious diseases, Parkinson's disease, autoimmune disorders, cancer, and recently even to COVID-19. The deficiency of this vitamin in the human body is defined with respect to the level of its major circulating metabolite, 25-hydroxyvitamin D (25OHD2 and 25OHD3), in the serum. A 25OHD level of 20-30 ng/ml indicates insufficiency, and below 20 ng/ml indicates deficiency. Current serum 25OHD detection techniques such as radioimmunoassay, liquid chromatography-mass spectrometry, and high-pressure liquid chromatography are expensive, time-consuming, and require trained personnel. Hence, there is a need for a reliable, cost-effective, point-of-care highly sensitive sensor for rapid quantification of vitamin D. Almost all of the reports on electrochemical sensors for Vitamin D detection deals with Vitamin D as a model analyte, whereas real-time applications require the detection of 25OHD. In the present work, we have developed a silver/silver oxide nanoparticle decorated carbon nanotube modified electrode for antibody-free, sensitive detection of 25OHD. The structure and morphology of the synthesized composite have been analyzed by different characterization techniques. The sensing mechanism and analytical parameters obtained using the electrochemical method are discussed. The performance of the present sensor in real samples (human serum) is also evaluated and discussed.

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P2.032 Flow dynamics in triply periodic minimal surface (TPMS) porous materials using MRI

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3D printing for the manufacturing of porous materials suitable for industrial applications may have significant advantages over current engineering approaches. In the case of heat exchangers, triply periodic minimal surface (TPMS) [1, 2] structures may outperform conventional solutions due to their regular and intertwined channel structure.

Magnetic Resonance Imaging (MRI) can be extended to monitoring fluid flow non-invasively in porous materials on microscopic length scales [3]. This unique capability is used in this study to characterise the flow dynamics of pore fluid and to identify flow features that serve to enhance heat and mass transfer.

Here we present measurements of fluid flow through the network of Schwarz Diamond TPMS. We initially report our previous results for Reynolds numbers between 1 and 32 [4], and then extend these up to a Reynolds number of 1000. We use specialised MRI pulse sequences that minimise artefacts caused by the tortuous flow, thus ensuring high quantitative accuracy in our measurements. We find that the regular channel shape inhibits preferential flow channelling that is problematic for random channel networks. We also find that the transverse flow pattern exhibits free shear layers in the channel centres that are associated with turbulent motion. These findings indicate that TPMS devices are suitable for enhanced heat and mass transfer because the turbulent self-mixing disrupts the boundary layer. The absence of channelling means that the entire channel network is utilised effectively, which is critical for applications where compact devices are required.

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P2.033 Exploring the Non-Classical Properties of Protein Structure

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The fibrous proteins collagen and spider silk share a unique functional similarity that is more commonly found in non-organic crystalline materials. Both proteins produce electrical charges in response to applied stress, demonstrating piezoelectricity. Collagen and silk have similarities in structure, such as having a rich glycine peptide sequence and secondary helical structures. However, the origins behind the piezoelectric response for each protein are assumed to be different.

In collagen, the triple helical morphology of tropocollagen and their quasi-hexagonal arrangement to form a fibril are said to be the main contributors to its piezoelectricity.[1], [2] However, for silk fibres, even though they also have helical motifs, the piezoresponse has been found to be mainly from the beta sheets that are present.[3] A study on the origins of piezoelectricity in silk has shown that by increasing both the beta-sheet content and crystallinity, the piezoelectric response has increased as well.[3] Other proteins such as elastin, keratin, and the globular protein lysozyme are piezoelectric but still lack understanding behind the mechanism.

The project aims to develop a structure-function relationship between proteins and their piezoelectric response. We will present how the piezoelectric response of different proteins vary with changes in their secondary structure. The presentation highlights the preparation of protein films with systematic variation of the secondary structure and results obtained through piezoresponse force microscopy on prepared protein films which include silk fibres with different helical/beta-sheet ratios and amyloid fibrils of lysozymes and hemoglobin.

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P2.034 Advanced Integral Magnetometry of Miniscule Powder Specimens and Thin Layers on Bulky Substrates

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We report two experimental methods that greatly minimize the experimental artifacts associated with mounting specimens of both solid flat-plate shape [1] or amorphous (miniscule biological, chemical, and powders) [2] for the standard DC volume magnetometry. In these cases the sought very weak signal is buried in the magnetic response of the substrate or a carrier (a capsule), therefore can be substantially contaminated by signals brought about by the chosen sample mount and magnetometer's instabilities. We show how in situ magnetic compensation (on the sample holder level) reduces the spurious and unwanted signals that originate from the bulky crystalline substrates or polycarbonate/gelatin capsules, respectively. These two concepts, are based on an elementary approach, in which this large error-bringing necessary signal from the specimen carriers gets reduced dozens of times by substantially restoring the translational symmetry of the whole samples holder, that is otherwise broken by the presence of any of these carriers. As the result the output is much less dependable on the inevitable fluctuations of some environmental variables, which detrimentally reduce the real credibility of the outcome in the standard approach to precision magnetometry. Additionally, a two- to five-fold reduction in the absolute noise level has been observed. Importantly, the solution proposed here can be easily incorporated in any magnetometer, in particular in Quantum Design MPMS and MPMS3 models. Importantly, the method requires neither any modelling of the magnetometer output signal, nor any laborious fitting.

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P2.035 Scattering simulations for Bessel beams near a plane substrate in the framework of the discrete dipole approximation

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Bessel beams are prominent examples of structured light possessing features valuable in diverse areas of photonics and medical science. First of all, ideal Bessel beams are diffraction-free, so they can propagate without intensity divergency along the propagation axis. Next, Bessel beams have a helical phase proportional to orbital angular momentum. Both of these qualities make Bessel beams a versatile tool for optical manipulation, holography, material processing, and many other applications. Various applications of such beams require the consideration of their scattering by particles and the contribution of a substrate. We report the simulations of vector Bessel beam scattering by particles near a substrate using the discrete dipole approximation. To implement the simulation of the Bessel beam scattering by particles near a plane substrate, we presented Bessel beams as a weighted sum of plane waves using the angular spectrum decomposition method. This allowed us to use the previous realization of plane-wave scattering near a plane substrate in the ADDA code (https://github.com/adda-team/adda). We also extended existing descriptions of different Bessel beam types using the angular spectrum decomposition method for all known Bessel beam types. The beta version of the code for the simulation shows good computational results and accuracy. Further development of the code will be valuable for the simulation of a wide range of experiments with Bessel beams involving the presence of a substrate.

P2.036 Electronic properties of 1T–TiSe2, numerical models of the formulation and melting of the charge density wave state

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The charge density wave (CDW) is an example of a low temperature phase of matter which occurs due to strongly correlated electrons. CDW materials are characterised by a periodic distortion of the atomic lattice, periodic modulation of the electronic charge distribution, and a complex order parameter. These materials have potential application in mechanical vibration detectors, optoelectric devices, information processing, memory, and many other next generation technologies. Many strongly correlated materials show non-trivial phases at similar temperatures and energy scales, and because of this, disentangling the mechanisms behind the phases has historically proven difficult using standard many-body methods. Here we use dynamical mean-field theory (DMFT) [1] in conjunction with density functional theory (DFT) and time-dependent Ginzburg–Landau (TDGL) formalism [2] to investigate the electronic properties of the CDW material 1T–TiSe2. Using these numerical techniques, we can understand both the formation of the CDW state and the melting of this phase due to the application of laser pulses and the resulting heating of the phononic environment.

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P2.038 Pyrolysed cobalt-based Macrocycles for the Electroreduction of CO2

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Converting CO_2 into materials such as chemicals or biofuels synfuels is an attractive way to mitigate greenhouse gas emissions while producing value-added products. Even though the intrinsic chemical stability of CO_2 significantly limits its reactivity, the usage of electrocatalysts allows its efficient reduction in a mild environment and at relatively low overpotentials. Cobalt phthalocyanine (CoPC), cobalt tetra-phenyl porphyrin (CoTPP), and Vitamin B12 (VB12) are well-defined Co-N4 macrocycles whose incorporation into heterogeneous catalysts setups has led to materials with outstanding CO_2 electroreduction reaction (CO_2ERR) properties, most notably in the selective formation of CO at high current densities.
These Co-N_4 macrocycles have also been used to manufacture catalysts efficient for the oxygen reduction reaction. Notably, the pyrolysis of the macrocyclic precursors supported by carbon materials allowed the fabrication of heterogeneous ORR catalysts with high loadings of catalytically active components, controlled local environments, and enhanced stabilities. While these properties could also lead to these materials being efficient catalysts for the CO_2 electroreduction reaction, to the best of our knowledge, such pyrolyzed catalysts have not been investigated for the CO_2ERR.
In this work, we report materials based on CoPC, CoTPP, and VB12, supported by carbon black and pyrolyzed under argon, as efficient catalysts for the CO_2ERR. The catalytic precursors were dispersed on carbon powders with ball-milling before being annealed at different temperatures based on the positions of the significant steps and plateaus thermal states of the pure precursor observed by thermogravimetric analysis of the pure precursors.

P2.039 Fine Tuning of Electronic Excited States in Donor-Acceptor Dyes; Steps Towards Designer Compounds for Modern Technologies.

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Donor-acceptor dyes are an integral part of modern chemical materials exhibiting unique photophysical properties, such as the electronic charge transfer (CT) transition. This displaces electron density throughout the structure of a compound. A behaviour which can elicit desirable properties that are used in many modern technologies including, solar cells,1 OLEDs,2 and molecular sensors.3 One of the most important aspects for these dyes in each application is the energy at which the electronic CT occurs. Hence, predictable tuning of this feature towards desirable wavelengths would be useful for the design and fabrication of future compounds used in these technologies. Often research will compare the discrepancies between different donor or acceptor moieties in efforts towards CT tuning. However, a much more subtle and controlled approach is to alter the substitutions or linkages within these units.4 Due to the localisation of the HOMO and LUMO frontier molecular orbitals to the donor and acceptor units respectively, adjustments to these groups can vary the energy of these two orbitals and hence the CT transition. Our investigation has looked into the subtle tuning properties of six donor-pi-acceptor dyes containing a carbazole donor and dithienothiophene bridging unit, bonded by meta or para linkages, and three variations of an indane-type acceptor. These dyes indicate the controlled CT tuning which can be achieved by making these small alterations. Additionally, the dyes also exhibited other interesting excited state characteristics, such as dual emission, high quantum yield and molar absorptivity, lending to potential uses in the afore mentioned technologies.

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P2.040 Robust Hybrid Ultramicroporous Materials (HUMs) for Efficient Gas Separation

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Metal-organic-frameworks (MOFs) are an attractive class of coordination compound well known for their highly porous nature. This property has made MOFs ideal candidates for applications, such as gas separation, sensing and storage. Recently, hybrid ultramicroporous materials (HUMs), a subfamily of MOFs that utilises inorganic pillaring units (SiF_6^{2-}, TiF_6^{2-}, GeF_6^{2-} etc.) have emerged as benchmark materials for gas separation processes. Driven by small pore sizes (< 7Å) and strong electrostatic interactions between pillaring units and guest molecules.[1]

We herein report the synthesis of novel HUMs for the application of gas capture and separation. These materials have been systematically designed to combine strong binding sites with fine-tuned pore windows to enable improved recognition and favourable uptake of specific gases. Single component adsorption and experimental breakthrough studies reveal the potential of these new hybrid materials to separate gases that are globally and industrially challenging (e.g.CO_2/N_2, CO_2/C_2H_2, C_2H_2/C_2H_4).[2,3] Furthermore, the novel materials were also found to be thermally and hydrolytically robust while also being able to carry out separations at a lower energy requirement.

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P2.041 Development and Application of Self-sealing cFET Valves to Capillary Circuits for Commercial Applications

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A novel approach for microfluidic capillary circuits is presented that holds the potential for massively improving commercial applications. Microfluidics open new avenues into performing previously difficult, time-consuming, or costly analysis in a more efficient and economical manner. Of increasing interest, the subcategory of channel-based capillary microfluidics (capillary circuits) uses the interfacial energy of a liquid/solid boundary to autonomously manipulate liquid flows [1]. The automated nature of capillary circuits mean they can provide simple, low-cost, lab-on-a-chip solutions in industries such as medical diagnostics and biological research.

However, capillary circuits are difficult to design due to the low flow control inherent in the autonomous nature [2]. While possible to use external control like pumps and valves, these increase cost and complexity, removing the benefits of microfluidics and reducing potential impact. Fully autonomous capillary circuits have all control encoded via the design of predefined microstructures, with the only manual action being liquid addition and result reading. The development of the capillary Field Effect Transistor (cFET) has broadened the range of flow control possible in capillary circuits and thus opened new opportunities for advanced applications [3–6]. This paper presents an overview of the cFET function and design developments, which improve cFET functionality and applicability.

Also discussed is the potential for commercial impact through the development of capillary circuits for specific applications. The low-cost, low-reagent, and low-training requirements make capillary circuits ideal for high-throughput testing of high-value samples in situations where a quick, easy result is favoured, particularly in healthcare or industrial production [7,8].

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P2.042 Electrocatalytic Reduction of CO2 to C2+ Compounds on Oxide-Derived Copper Nanoparticles

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As the need to remove carbon from the atmosphere grows ever larger due to the desire to fight climate change increasing, the electrochemical reduction of carbon dioxide to value added products, such as CO, C2H4, and C2H5OH proves a promising option to not only remove CO2 from the atmosphere, but also produce the aforementioned products without using fossil fuels [1]. Copper has long proved a popular catalyst for the CO2 reduction reaction (CO2RR) as it is the only known pure metal to reduce CO2 to products that require more than two electrons, such as C2H4 and C2H5OH, at reasonable faradaic efficiencies [2].

We have developed a novel oxide derived copper nanoparticle (OD-Cu) electrocatalyst which can reduce CO2 to C2H4 and C2H5OH, with good selectivity and high activity, that is typically reserved for gas diffusion electrodes. Here, we show the impact that various factors such as loading, applied potential and calcination temperature have on the selectivity and activity of the OD-Cu catalyst.

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P2.043 Nano-diamond Coated Carbon Fibers for improved Dopamine Sensing Applications.

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Neurotransmitters are chemicals associated with neuronal synapses that are involved in psychological processes such as learning and memory. Their pathologies are correlated with many neurological disorders like depression and drug addiction. Electrochemical methods such as Fast Scan Cyclic Voltammetry (FSCV) are the only technique for measuring neurotransmitter levels in real time [1]. However, it is extremely challenging to construct an electrode that can perform these measurements long-term. Carbon fiber electrodes have been used for electrochemical detection of neurotransmitters for a long time [2, 3]. Compared to conventional metal electrodes, carbon fibers are thin and flexible, and therefore avoid the hosts immune response that limits traditional electrodes over time. Carbon fiber has shown limited ability in chronic neurotransmitter detection due to the degradation of the fiber over time at the stimulation voltages required for their measurement [4]. This study aims to increase the capabilities of carbon fibers for chronic neurotransmitter detection using doped Ultra-Nano Crystalline Diamond (NUNCD) or Carbon Nano-Wall (B-CNW) coatings [5]. We deposit these coatings on carbon fiber using microwave-plasma enhanced chemical vapor deposition. Our results show that these coatings can improve the electrochemical properties of the electrodes. FSCV using these electrodes show sensitivities for dopamine detection higher than bare carbon fibers. Along with the larger water window it is expected that these coatings will aid in the long-term stability for neurotransmitter sensing. Our newly developed electrodes will be suitable for robust, chronic detection of neurotransmitters in real-time, and will be valuable in the research and treatment of neurological disorders.

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P2.044 Surface Passivation Strategies for Colloidal Quantum Dot Solar Cells

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Colloidal quantum dot (QD) solar cells have emerged as a promising low cost, low embodied energy and high-efficiency photovoltaic technology. Since 2008, cell efficiencies have increased from 2% to 18% in 2022 [1,2]. Among QD solar cells, Pb chalcogenide QDs stood out due to their high efficiency, simple fabrication process and good stability. PbS QD cells having a record efficiency of 13.8% have been demonstrated [3]. Due to the quantum confinement effect, the bandgap of the material is size dependent, enabling optimized-bandgap single-junction cells and multi-junction tandem devices.

The rapid development of colloidal QD solar cells is attributed to the great research efforts leading to the advancement in materials synthesis, surface passivation, and device fabrication. Our research has been focused on surface passivation to improve device performance in terms of both efficiency and stability. Examples include the development of an effective passivation route for PbSe QDs using lead halide perovskite nanocrystals as Br- or I- sources. This approach has significantly reduced surface defect density as evidenced by enhanced PL quantum yield (PLQY) [4], leading to an efficiency over 10%, the highest for PbSe QD cells [5]. Surface passivation strategies for PbS QDs have also been developed including incorporating a thin alloyed shell on their surface leading to very high PLQY (>85%), as well as incorporating KI3 in the ligand exchange process enabling an efficiency of 12.1% [6]. In this presentation, details of above novel passivation approaches developed by our research team for improving QD solar cells will be presented.

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P2.045 Time-dependent Transient Nonlinearity In Silicon Nanostructures

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Nonlinear silicon nanophotonics has attracted great interest for the efficient enhancement of optical nonlinearity, which originates from the plethora of electric and magnetic Mie resonances. Our group recently discovered giant optical nonlinearity based on photothermal effects in silicon nanostructures, whose nonlinear index n_2 presents a five-orders enhancement compared with bulk silicon [1].

Conventionally, intensity-scan methods such as z-scan or x-scan techniques are employed to examine the nonlinear behaviors between input intensities and output signals in the spatial domain, while their temporal characterization relies on the pump-probe techniques.

Here, leveraging the combination of spatial x-scan and temporal pump-probe techniques on silicon nanostructures, we unravel unconventional time-dependent transient nonlinear behaviors, where the underlying mechanism is based on nonlinear carrier dynamics with their fluence-dependent carrier lifetime [2]. This phenomenon is exemplified through the nonlinear Auger process. Auger-induced transient nonlinearity is not only located at several tens of picoseconds delayed time, but also presents diverse nonlinear behaviors, including sub-linear, super-linear, and surprisingly full saturation. Moreover, we unraveled a “crossing point” in the pump-probe traces, where the probe remains constant as pump-fluence increasing. As sublinear and super-linear fluence dependencies result in single-particle image broadening and shrinking, transient nonlinear was then applied to point spreading function engineering, further confirming the nonlinearity as well as demonstrating the potential of sub-diffraction microscopy.

We believe that this demonstration provides the general scenario of transient nonlinearity generation and the presented Auger-based mechanism is generally applicable to other semiconductor nanomaterials, which benefit applications in all-optical signal processing and super-resolution imaging.

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P2.046 Coating-free Surface-tension Gradient Networks for Condensing Heat-transfer Surfaces

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Condensation and frosting are common phenomena across many heating, ventilation, and air conditioning (HVAC) systems. Surface coverage of condensation or frost presents a heat transfer resistance between the surface and surrounding environment, often an integral component of system operation. A reduced need to defrost and/or remove condensation from heat transfer surfaces reduces energy expenditure and thus increases the efficiency of the system. As such, the development of heat transfer surfaces with anti-frosting qualities has become an area of interest [1] [2].

In the present work, aluminium surfaces with coating-free topographical networks of surface tension gradients, inspired by nature [3], are investigated for their microdroplet growth mechanisms, frost wavefront propagation velocity, and heat transfer coefficient. Previous work found that in-plane forces acting on droplets with sub-capillary length diameters result in spontaneous droplet motion, or aid in surface defrosting [4]. It is thought that this will enhance surface water management by removing condensed droplets at smaller radii and hinder frost wavefront propagation across the surface, making the surfaces useful for heat exchangers.

We present results from our experimental investigations into condensation and frosting on these surfaces. We will first describe the construction of a subsonic wind tunnel to produce controlled condensation and condensation-frosting conditions, together with image processing methodology that allows the generation of growth curves that track average droplet radius and surface droplet concentration over time, similar to literature [5]. We will present preliminary results of growth curves and frost wavefront velocities on a variety of surfaces, including surface tension gradients.

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P2.047 Optically Active Quantum Dots on Plasmonic Resonators for Visible Light Hydrogen Photocatalysis

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Plasmonic resonators can highly concentrate optical energy into ultra-small volume that has dimensions far below the wavelength. [1] When coupled with optically active materials, e.g. quantum dots (QDs), plasmonic resonators can be used in numerous applications like photovoltaics and photocatalysis. [2] This is because the resonators can provide extreme optical concentration and, in some cases, inject additional hot electrons into the materials. This then leads to enhanced generation of photocarriers and elevating performance in relevant applications.

Here we report the coupling of large-area plasmonic resonators with optically-active QDs for enhanced hydrogen photocatalysis. Specifically, we have fabricated cm2-scale silver nano-gratings using interference lithography which are then integrated with Cadmium Selenide (CdSe) QDs. The angle-resolved reflection revealed the resonant illumination conditions for excitation of plasmon resonances. These conditions are used for angle-resolved photoluminescence experiments resulting enhanced absorption/emission in the QDs with a factor of ~ 1.5. This enhancement to the pump absorption in QDs (Purcell's enhancement) generated more carriers hence elevated the detected photocurrent by similar order of magnitude (~ 1.1) which is confirmed from linear sweep voltammetry. These results show promise for enhancing photocatalytic reaction rates in Plasmonically coupled semiconductors for direct solar-to-H2-production.

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P2.049 Reversible Voltage Control of Magnetic Anisotropy by Ionic Liquid Gating in MgO/CoFeB/W Stack for Voltage Tuneable Magneto Resistive Sensor

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This study aims to fabricate a voltage-tuneable magneto resistive sensor with the ability to measure small magnetic field signals in three dimensions. Sensing direction in magneto resistive sensors is linked to the magnetization of reference layer. Materials like CoFe1, CoFeB2 and Heusler alloys3 are good choices as reference layers due to their adjustable magnetic anisotropies. Here, using ionic liquid gating (ILG), we observed that magnetic anisotropy of reference layer CoFeB is switchable in MgO(1.5nm)/CoFeB(1.6nm)/W(0.5nm) stack. We used ionic liquid N, N-diethyl-N-methyl N-(2-methoxyethyl) ammonium bis (trifluoromethylsulfonyl) imide (DEME TFSI) (IoLiTec) for applying the gate voltage (VG) ranging between ±3.5V. Using the magneto-optical Kerr effect, we have investigated the change of anisotropy using different gate voltages. We found that magnetic anisotropy switches from out-of-plane (virgin state) to in-plane upon the application of +3.5V, whereas removal of applied voltage +3.5V or application of -3.5V, switches magnetic anisotropy back to out-of-plane, demonstrating the switching behaviour of the stack is reversible and repeatable. Moreover, we observed that out-of-plane to in-plane anisotropy switching time is higher (~45 sec) compared to in-plane to out-of-plane switching time (~25 sec). Hence, a stack having stronger out-of-plane and switchable anisotropy is ideal to use in voltage tuneable magneto resistive sensors.

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P2.051 High voltage-durable electrolyte system for multivalent-ion supercapacitors

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Supercapacitor is considered one of the most promising energy storage system devices that can deliver high power density, long cycling life and safe operation, and is composed of an ideally polarized electrode pair (IPE) and an ionic charge carrier in a solvent system. Charge carriers stabilized by solvent molecules in an electric field become polarized and gather on the IPE surface to form electrochemical double layers (EDL). Physisorption capacitance is proportional to the electrochemically active surface and inversely proportional to the distance between the IPE and the charge carrier. For this reason, previous studies of supercapacitors focus on two major issues: increasing the surface area of IPE and creating well-tuned pore structures based on optimized electrode material properties. However, the charge storage capacity of nanoporous carbons was mainly investigated in monovalent charge carriers. Despite advances in the understanding of monovalent ion-based capacitors, multivalent ion charging behaviour, especially of nanoporous carbons, remains inadequate. Multivalent ions with small ionic radii, such as magnesium ions, are significantly affected by solvation sheaths and strong ionic interactions with solvent molecules. This affected the redox potential of the electrolyte as well as the EDL configuration. Moreover, the Debye length of multivalent ions is longer than that of monovalent ions with similar ionic radii. Debye length and ionic interactions are important factors for capacitive charge storage capacity, especially in nanopores. Because EDL capacitance arises from tuned nanopores. In this case, a limited number of charged carriers are inserted into the superionic state nanopores. This study aims to evaluate the capacitive Mg ion charge of nanoporous carbon, various organic solvents such as dimethoxyethane (DME), acetonitrile, dimethyl carbonate, and propylene carbonate. Multivalent ions such as calcium ions and alkali ions with different ionic radii were evaluated for comparison under the same electrochemical state. Different nanoporous carbon structures of ultra-mesoporous carbon and microcarbon structures were evaluated for the effect of pore size. These systematic studies revealed that the capacitive charging behaviour is highly dependent on the pore structure of the charging carrier, solvent and electrode material. In conclusion, systems based on DME electrolytes with smaller multivalent Mg ion-charged carriers have wide and stable operating ranges below 4 V due to strong ionic interactions between DME and Mg.

P2.052 A New Type of Conformal Fractions Binder Bolstering Electrochemical Performance: Toward Flame Retardant High-power Lithium-Sulfur Flexible Batteries

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Here, we report for the first time the use of tragacanth gum binder (containing essential functional groups like amine, hydroxyl, and carboxyl) for the preparation of highly mass-loaded sulfur as positive electrodes for Li-S batteries. The tragacanth family consists of more than 3000 species, where our study selectively demonstrates the use of tragacanth gum that contains high content of components such as fucose, rhamnose, arabinose, and nitrogen-containing components like hydroxyproline influencing capacity retention and stability in Li-S batteries. We have found that the macromolecular biopolymer, Tragacanth gum, inherits heterogenous polysaccharide fractions, which satisfy four critical prerequisites as an ideal binder for a better operation of high-performance Li-S battery. 1) TG binder enables high access for Li-ions to sulfur-active particles (up to 80.3% of S) through the anionic polymeric backbone moieties triggering efficient sulfur reactivity. It was adjustable to house high sulfur loading over 12 mg cm-2 without compromising the sulfur utility and reversibility. An important point to be noted is that our "gelation" method (less amount ≤ 5% of binder in electrode) is equivalent to the current industrial standard Li-ion battery electrodes (LiCoO2, Li-NMC) which use 6% of binder in the electrodes. 2) It exposed polar functional groups of saccharidic units expedite the trapping of soluble polysulfides (Li2Sn, n=4~8) into the electrolyte to maintain the electrolyte concentration, which this feature was theoretically supported through DFT calculations. 3) It actively regulates large volume changes through stretchable rod-like tragacanthin and sphere-like bassorin molecular conformations ensuring robust mechanical strength. The exceptional elasticity confirmed through nanoindentations kept the electrode's volume changes within 16%, even at 4 C. 4) Apart, the water-processable and fire-retardant ability of TG binder impart environmentally compliant and good thermal stability for safer Li-S batteries. Further, the flexible Li-S battery delivers a stack energy density of 230 Wh L–1 even in harsh conditions, demonstrating high reactivity of sulfur along with good shape conformality. The prospective findings from our study underpin multifunctional positive attributes of the TG binder in realizing high-performance, flexible and safer cathodes for Li-S batteries. Therefore, these definite improvements in the sulfur battery chemistries would pave the way to realize high-performance electrochemical energy devices for e-transportation, portable power electronics, and so on, considering the prevalence, cost-effective and sustainable characteristics of sulfur.

P2.053 Heterogeneous ion-exchange membranes fabricated with ionomer binder and nanofiber

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Ion-exchange membrane (IEM) is a key component that determines the performance of electro-membrane processes such as electrodialysis (ED), reverse electrodialysis (RED), and continuous electrodeionization (CEDI) [1]. In order to improve the performance of the electro-membrane process, the IEM must have low electrical resistance, high permselectivity, and excellent physical strength. The IEM can be divided into two types, i.e. a homogeneous IEM and a heterogeneous IEM, according to their intrinsic structure. A homogeneous IEM in which fixed charges are evenly distributed has the advantages of low electrical resistance and high permselectivity but has the disadvantages of weak physical strength and high production cost. On the other hand, a heterogeneous IEM fabricated by mixing ion-exchange resin powder and an inert polymer binder has high electrical resistance and low permeation selectivity but possesses the merits of a simple manufacturing process and low production cost [2]. In this study, ionomer binder and nanofiber were employed to fabricate a heterogeneous IEM. Since the ionomer binder and nanofiber provide an ion transfer path, the ion conductivity could be significantly improved while the mechanical strength was also enhanced [3]. The performance of the heterogeneous membrane could be optimized by determining the optimal ratio of the ion-exchange capacity of the ionomer binder and the content of the ion-exchange resin powder. The prepared heterogeneous IEMs were applied to a CEDI process to confirm the performance of the IEM. This work was supported by the National Research Foundation of Korea (NRF) grants funded by the Korea government (MEST) (NRF-2019R1A2C1089286 and NRF-2022M3C1A3090848).

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P2.054 Organic-inorganic composite all-solid electrolytes with high ion conductivity improved through electric field alignment

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An electrolyte is an essential component that determines the performance of electrochemical devices. Since high ionic conductivity is required, organic liquid electrolytes are mainly used in most applications including secondary batteries. However, although liquid electrolytes have the advantage of high ionic conductivity, they also cause problems related to stability such as leakage, evaporation, and flammability, which leads to degradation of electrochemical device performance [1]. On the other hand, all-solid electrolytes possess excellent electrochemical and physical stability as well as high energy density [2]. An organic polymer electrolyte, one of the all-solid electrolyte types, has the advantage of being flexible and able to adhere to the electrode and interface but has a disadvantage in that it has low mechanical strength and ionic conductivity [3]. In addition, inorganic solid electrolytes have relatively high ionic conductivity and high mechanical strength, but have low interfacial stability due to their rough surface [4]. In this study, therefore, an organic-inorganic composite all-solid electrolyte was developed to complement the disadvantages of these organic polymer electrolytes and inorganic electrolytes. In particular, by controlling the properties of the polymer, the mechanical properties of the all-solid electrolyte and the affinity with the electrode were improved, and the ionic conductivity could also be improved through the alignment of the nano-sized inorganic filler under a strong electric field. This work was supported by the National Research Foundation of Korea (NRF) grants funded by the Korea government (MEST) (NRF-2019R1A2C1089286 and NRF-2022M3C1A3090848).

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P2.055 Photocatalytic Performance of Mono and Bimetallic Ag, Au Decorated CN: Effect of Semiconductor and Surface Plasmon Excitation Synergy

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Maximizing the solar-to-chemical photoconversion efficiency is a major hurdle in the domain of heterogeneous photocatalysis. With regard to photocatalytic processes for resolving energy and environmental issues, the combination of semiconductor and plasmonic metal nanoparticles (NPs) has been practiced adequately. We have decorated gold (Au) and silver (Ag) NPs over graphitic carbon nitride (g-C3N4 or CN) nanosheet and examined the activity of the catalysts under UV-visible irradiation with rhodamine B (RhB) dye as the model pollutant. UV-visible radiation triggers a synergy in excitation of both the semiconductor and metal NPs. Consequently, we encountered a diminished photocatalytic activity in metal NPs decorated CN [1]. We have further advanced our study with Ag and Au bimetallic decorated CN (AgAu/CN). The possible charge transfer pathways and mechanism is illustrated under UV-visible light irradiation [2]. Thus, in this work, we present the comparison between photocatalytic activity of mono and bimetallic Au, Ag decorated CN. For the initial investigation of the synthesized materials, various characterization tools are used, such as X-ray diffraction (XRD), transmission electron microscopy (TEM). Photoluminescence (PL) spectroscopy and diffuse reflectance (DRS) spectroscopy are employed to study the optical properties. The charge carrier dynamics is analyzed with time-resolved PL (TRPL) spectroscopy. The surface characterization is done with X-ray photoelectron spectroscopy (XPS). Finally, the regulating mechanism for the photocatalytic degradation process is proposed to be the collective charge carrier transfer from CN to metal and metal NP to CN. The dominance of FRET (Forster-resonance energy transfer) over PIRET (plasmon-induced resonance energy transfer), interfacial trap centers and reduced optical field intensity at the bimetallic gap are marked as the contributing factors for the overall photocatalytic activity [2].

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P2.056 Self-assembled Peptide Porphyrin Nanofibers as Cheaper Light Harvesting Systems

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Cheap artificial light harvesting systems, which competently harvest solar energy and promote efficient energy transfer, are highly sought after in the renewable sector. This research reports the synthesis of self-assembled peptide-porphyrin fibers (SJ 6) fabricated with magnetic iron oxide nanoparticles as feasible electron acceptors (SJ 6-nFe3O4). Charge-complementarity between the negatively charged peptide (20E) and the protonated Zn-tetraphenyl porphyrin (ZnTPyP) led to an ordered assembly of the ZnTPyP molecules enabling efficient light harvesting. XRD data indicates a more ordered structure in SJ 6 compared to 20E and ZnTPyP. The photophysical analyses of SJ 6 suggest - excitonic coupling between porphyrin molecules in SJ 6. The incorporation of Fe3O4 nanoparticles into SJ 6 was confirmed using transmission electron microscopy and a fluorescence quenching experiment. The SJ 6-nFe3O4 system performed the light reaction of photosynthesis as confirmed by the reduction of 1 mM NAD+ to 0.180 mM NADH upon exposure to visible light (Xe lamp > 420 nm) for 1 h. The photochemical regeneration of NADH using the SJ 6-nFe3O4 system was coupled to glutamate dehydrogenase catalyzed conversion of a- ketoglutarate to L-glutamate. These results confirm the successful synthesis of an artificial light harvesting peptide-porphyrin system with Fe3O4 nanoparticles as promising low cost electron separators.

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P2.057 Preparation of Highly Stable Perovskite Quantum Dots by B-site Passivation

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Due to the ionic-nature of perovskite quantum dots, defects in core and surface of perovskite QDs are easily generated during and after synthetic processes. X-type ligands including thiol functional groups can effectively passivate halide vacancies and simultaneously bind with uncoordinated B sites. In this study, a novel synthesis method for defect-psssivated core-shell perovskite QDs by using thiol-based ligands are investigated.

P2.058 Modelling transport properties of a transverse magnetic focusing system with spin-orbit coupling

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Spintronics, where spin is manipulated instead of charge to transfer and store information, is a promising field that can deliver energy efficient devices. Spatially separating carriers of different spins and efficiently generating spin currents are crucial steps towards building practical spintronics devices. Transverse magnetic focusing (TMF) is a potential technique to accomplish both those tasks. In a two dimensional material where there is significant Rashba spin-orbit interaction, electrons or holes of different spins will traverse different paths in the presence of an external magnetic field (Fig. 1). Experiments have demonstrated the viability of this technique by measuring conductance spectra that indicate the separation of spin-up and spin-down carriers. However, there are physical effects that are still not well understood. We utilise finite difference and the non-equilibrium Green's function (NEGF) formalism to calculate transport properties of TMF devices using the software KWANT. [1] By doing so, we analyse the effects of varying conditions such as spin-orbit coupling, magnetic field, device geometry, and disorder strength. [2]

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P2.059 Using catalytic transesterification for synthesizing aromatic-aliphatic copolymers by melt blending

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In New Zealand, approximately eight thousand tonnes of PET waste are landfilled annually. Transesterification offers an alternative way of repurposing this waste compared to traditional recycling methods, which have their limitations in dealing with the wide variety of PET wastes. Through transesterification, PET waste can be recycled by copolymerizing with aliphatic polyesters such as polycaprolactone (PCL) to create novel biodegradable polyesters. One of the most critical factors that have been overlooked is the impact of the randomness of copolymers on biodegradability. This study assesses the effectiveness of producing a random copolymer using nuclear magnetic resonance spectrometry, differential scanning calorimetry, and gel permeation chromatography. By blending PET and PCL at 280°C under a nitrogen atmosphere, a randomized copolymer with a single glass transition temperature was created in the presence of 1wt% titanium butoxide catalyst. Both the metal ions' acidity and nucleophilicity of ligand are crucial to achieving a high degree of transesterification. Another popular transesterification catalyst, dibutyl Tin (IV) oxide, did not show high activity towards transesterification. Varying blending times between two and ten minutes using titanium butoxide resulted in comparable copolymer yield, suggesting the process is compatible with an extrusion process. In contrast, the extent of transesterification scales positively with the amount of titanium butoxide catalyst added, and the minimum amount of catalyst required to form a randomized copolymer is estimated to be about 0.5wt%. This study's results will help identify the catalytic mechanism and customize an effective and non-hazardous catalytic process for transesterification between polyesters.

Keywords: PET recycling, transesterification catalyst, aromatic-aliphatic copolymer

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P2.060 Smart membrane with permeate flux control through a redox switch

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The permeate flux control through a smart filtration membrane, using a pH or temperature switch, has been of a significant interest in the recent years. However, both stimulus could cause possible composition changes of permeate in the beverage filtration and clarification. A redox active coating on a filtration membrane could provide a redox switch as an alternative for the permeate flux control with the least effect on the beverage's quality. In this work, we modified a polyethersulfone (PES) microfiltration membrane with poly(3,4-ethylenedioxythiophene) (PEDOT) coating through vapour phase polymerization. The conductive membrane (PES/PEDOT) showed a good performance in both permeate flux and electrical conductivity after optimizations on the polymerization parameters. The redox activity of the PEDOT coating was investigated by Raman spectroscopy mapping. A flux switching behaviour was observed after oxidizing and reducing the PEDOT coating. The counterion migration into and out of the PEDOT coating is considered to be the key mechanism for the flux control behaviour observed during the redox cycle. The conductive PES/PEDOT membrane provides a new redox switch option for the permeate flux control in beverage filtration systems.

P2.061 Near-infrared organic light-emitting diodes with thermally activated delayed fluorescent host sensitization.

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Near-infrared organic light-emitting diodes (NIR-OLEDs) with emission wavelengths greater than 750 nm can realize applications such as bioimaging,[1] biomonitoring,[2] and optical communication.[3,4] However, near-infrared light-emitting molecules are limited by non-radiative loss resulting in low light-emitting efficiency. In our previous study, the Förster resonance energy transfer (FRET) process between the exciplex co-host to the infrared emitter was reported to improve the external quantum efficiency (EQE) of a near-infrared device emitting at 774 nm up to 5.3%.[5] However, current exciplex systems have struggled to match the absorption profiles of longer emission wavelength emitters. Thus, we propose a spectrally matched host-sensitizer-emitter ternary light-emitting layer configuration to realize the FRET process. In this study, the thermally-activated delayed fluorescent (TADF) emitter DMAC-TRZ with greater than 80% quantum yield in neat-thin-film emissive layer condition was chosen as the emissive layer host.[6] Also, we used two newly synthesized emitters, Red-1, and NIR-1, in which the red fluorescent emitter Red-1 has a high quantum yield as a sensitizer and NIR-1 with an emission wavelength of 820 nm as an infrared emitter. Finally, we realized a NIR-OLED with an emission wavelength of 821 nm and an EQE of 1.5%. Such results indicate that FRET sensitization can be considered a potential strategy for NIR emission.

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P2.062 Nanoscale polarization control in oxide heterostructures studied via infrared and confocal Raman spectroscopy

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The interface of complex oxide heterostructures, such as SrTiO3 or KTaO3 with LaAlO3 or AlOx, is of great current interest because it presents a large platform to study unusual phenomena like the metal/superconductor-to-insulator transition [1] or the electrical modulation of the spin-orbit Rashba coupling for spin-charge conversion [2].

Here, the interface and bulk polarization phenomena in materials are investigated with a combination of confocal Raman and infrared spectroscopy, which function as complementary techniques. For instance, it was found that an important role in SrTiO3-heterostructures is played by a polar lattice distortion that is non-collinear, highly asymmetric and hysteretic with respect to the gate field [3]. This polarization can however depend on the material's domain pattern and on its vicinity to the ferroelectric quantum critical point [4].

These findings open new perspectives for the defect engineering of e.g. lateral devices with strongly enhanced and hysteretic local electric fields that can be manipulated with various parameters, like strain, temperature, or photons.

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P2.063 Redefining the Electrochemical Kinetics of Redox Reactions on Passive Surfaces.

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The mechanisms for redox reactions occurring on metal substrates generally assume a bare metal surface but bare metal surfaces only exist at sufficiently negative potentials (e.g., for Pt < -0.15 VSHE). At higher potentials, the surface is covered with a point-defective, barrier oxide layer (bl) upon which may exist a non-point defective, precipitated outer layer [e.g., Pt/PtO/Pt(OH)2. For Pt, the barrier layer is found to be an n-type semiconductor having the general formula Pt(1+x)O(1-y), indicating the presence of metal interstitials and oxygen vacancies. The surface vacancies are postulated to act as reaction sites at the barrier layer/solution interface and the surface oxygen vacancy has been postulated as providing the adsorption sites for the oxygen electrode reaction (OER) on passive titanium thereby linking the reaction mechanism to the defect structure of the substate bl oxide. However, the bl also represents a barrier to electron transfer. The theory of the electrochemical kinetics of redox reactions has been developed to accommodate reactions on passive surfaces and to involve surface point defects (primarily oxygen vacancies) in the reaction mechanism. The Point Defect Model (PDM) is used to calculate the surface concentration of the appropriate vacancy and to estimate the thickness of the bl as a function of voltage. The Generalized Butler-Volver equation is used to define the exchange current density in terms of the standard exchange current density for the reaction on the hypothetical bare metal surface as illustrated by the electrochemistry of carbon steel in hydrogenated alkaline solutions.

P2.064 Tailoring Perpendicular Magnetic Anisotropy of Heusler alloy thin films using Ion Irradiation

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Magnetic Tunnel Junctions (MTJs) are multi layered devices that use tunnel magnetoresistance to detect changes in magnetic fields. [1]. MTJs with specific characteristics are relatively complex to fabricate due to the high dependence of their magnetic properties, especially perpendicular magnetic anisotropy (PMA), on individual film thicknesses and interfaces. Post growth modification tools, such as ion irradiation [2], are thus needed to modify these properties. Ion irradiation is a versatile tool that causes structural changes and introduces disorders in the material's lattice by forming irradiation induced point defects [3]. These defects alter the magnetic properties which can be controlled by tuning the fluence, energy, and ion current density of the beam.

We report a study of changes to the magnetic properties of Sub-SiO2\Pd(2.5)/Co2MnGa(3)/Pd(2.5) stack with inherent PMA, when irradiated with 30 keV argon and neon ions at fluences between 10^{13} and 10^{15} ions/cm^2. The anisotropy of the magnetic layer was seen to change from out-of-plane to in-plane upon ion irradiation, even in the low fluence regime (<10^{14} ions/cm^2), with a hint of canted anisotropy. The Transport of Ions in Matter (TRIM) simulation [4] yields displacement per atom between 0.07 and 16.80 for fluences 10^{13} and 10^{15} ions/cm^2. Detailed experimental results obtained from Magneto-Optical Kerr Effect Spectroscopy and magnetometry supported by TRIM simulations will be presented in the conference.

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P2.065 Hydrogen reduction of raw and pre-oxidised NZ titanomagnetite ironsands in a small-scale high-temperature fluidised bed.

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Using hydrogen as a reducing agent can substantially reduce CO2 emissions from the ironmaking process. Several studies have reported sticking of particles when reducing iron ore fines in a fluidised bed using hydrogen at high temperatures (>800°C), whereby the particles agglomerate causing the bed to defluidise, effectively shutting down the process. Here we report that the reduction of NZ titanomagnetite ironsands in a small-scale laboratory fluidised bed (100 g) at temperatures between 800-1000°C using 100% hydrogen at flow rates up to 5 SLPM. No sticking phenomena are observed under these conditions, and this is attributed to the formation of a stable titanium-bearing oxide layer on the exterior of each particle which prevents iron-iron contact at the particle surfaces. Pre-oxidised NZ titanomagnetite ironsands have also been shown not to stick. Interestingly the reaction kinetics for pre-oxidised ironsands is faster at lower reduction temperatures when compared to raw ironsands. The increased kinetic rate can be attributed to the pre-oxidation stage inducing micro-fractures that create a void for the hydrogen to diffuse into the inner regions of the particle. The findings are important as increasing the operating temperature of the fluidised bed reactor results in a faster reaction rate and higher gas utilisation, making the process more economically attractive.

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P2.066 Synthesis of transition metal carbide nano-catalytic surfaces for hydrogen evolution reaction by ion implantation

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Platinum is the most effective electrocatalyst for the hydrogen evolution reaction (HER), however this noble metal is expensive. Transition metal carbides (TMCs) have the potential to be a low-cost alternative to platinum. In particular, tungsten and molybdenum carbides are promising as they mimic the electronic structure.1,2 Traditional TMC synthesis requires high temperature, which induces nanoparticle agglomeration consequently decreasing their electrochemical performance. Ion implantation offers a non-thermal equilibrium pathway to overcome the kinetic barriers in forming TMC nanoparticles at room temperature (bulk). In this work, we explore the ion implantation parameter space (mainly, energy and dose) extensively to identify the optimum conditions for forming most active molybdenum carbides phases (γ'-MoC and β-Mo2C) for HER.

Carbon was implanted into molybdenum thin films (~100 nm) at different implantation energies and fluences (10-20 kV and 2.5-25x1016 at/cm2). X-ray photoelectron spectroscopy confirmed formation of carbide in all implanted samples. Formation of different MoC phases including γ-MoC, γ'-MoC, η-MoC, β-Mo2C, β'-Mo2C were identified using selected area electron diffraction from HR-TEM and GI-XRD. The catalytic activity of these phases is well understood from DFT and experimental results.1,2 The highest electrocatalytic performance was achieved for β-Mo2C formed by implantation at 20keV (energy) and a dose of 2x1017 at/cm2. An overpotential of 267mV was required to reach a current density of 10 mA/cm2 on atomically smooth substrates (roughness < 1.5 nm). Application of this implantation recipe into high surface area substrates is likely to result in significant improvements in their HER activity.

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P2.067 Chiral cages by template-directed narcissistic assembly

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Chiral cages by template-directed narcissistic assembly
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Cage architectures with a discrete inner cavity have been of long-standing interest.[1] The development of chiral cage molecules has experienced an exponential growth facilitating their potential application in chiral recognition, chiral catalysis, and host-guest chemistry. The incorporation of chirality into the cage can be achieved either by employing chiral linkers (ligands) or chiral capping ends. It is often noticed that templating has significance influence to construct complex architectures like cage.

The macrocycle resorcin[4]arene is well known for its concave cyclic array, facile synthesis from resorcinol and a aldehyde, and in the application of host-guest chemistry. 3-Methoxyphenol as a replacement of resorcinol gave birth to racemic tetramethoxy-tetrahydroxy resorcin[4]arene.[2] Further modification or extension on the upper rim of the cyclic array allows more space for guest binding by tuning the depth of the cavity and acting as a capping end of the cage skeleton. Herein, we explore the template directed synthesis and properties of the C4-symmetric chiral cage constructed from a chiral derivative of resorcin[4]arene via covalent bond formation.

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P2.068 Electronic and thermoelectric properties of chalcogenide doped copper iodide

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Energy efficient electronics yield enormous opportunity for the future device applications. Among them, transparent thermoelectric materials are promising for energy harvesting, on-chip cooling, photodetectors and infrared detectors. The efficiency of such a thermoelectric material is given by its dimensionless figure of merit, $ZT=\alpha^2\sigma T/\kappa$ where σ is the electrical conductivity, α is the Seebeck coefficient, κ is the total thermal conductivity, and T is the operating temperature. Adversely interlinked α, σ and κ pose a major challenge due to complicated charge carrier dynamics dependent on the near band-edge electronic structure. To optimise the carrier concentration for increased thermoelectric performance, transparent copper iodide (CuI) can be substitutionally doped with chalcogenides (O, S, Se, Te) [2]. These defects show shallow ionisation levels and a strong preference for I-site occupation.

Tellurium was doped by ion implantation at 65 keV into CuI film [3] with fluences between 5×10^{14} and 5×10^{15} at/cm² which yield around 0.4 - 4.0 at% Te at an average depth of 20 nm. XPS and SIMS results showed successful Te doping into CuI. Seebeck measurements results showed a Seebeck coefficient near ~200μVK-1 at low doping fluences (≤1×10^{15} at/cm²), while at large fluences (≥2×10^{15} at/cm²) an anomalously large negative Seebeck coefficient is observed. The electrical conductivity for the 5×10^{14} at/cm² doped sample is 34 S/cm, yielding a power factor of 90 μW/mK². First-principles electronic structure calculations with Hubbard parameters are used to study defect properties in CuI:Te. Detailed electronic structure and thermoelectric properties of doped CuI will be presented at the conference.

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P2.069 Fibrosis, flexibility, and functionality: Totally internal cochlear implants as a case for what we miss when engineering for medicine

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For those with profound to severe sensorineural hearing loss, cochlear implants bypass damaged inner ear structures to directly electrically stimulate spiral ganglion neurons along the length of the cochlea to simulate hearing with typically positive outcomes [1]. Despite this, global adoption rates of cochlear implants are estimated at no more than 10% [2]. Totally internal cochlear implants (TICI) provide an avenue for increasing quality of life, decreasing hearing loss stigma, and promoting treatment uptake. A successful TICI design is yet to be published, despite numerous unique approaches in literature, primarily due to the difficulty of acoustic sensing within the inner or middle ear.

A prominent example is to utilise piezoelectric micro-oscillators operating at a resonance response to mechanically amplify signal compared to conventional flat-band responses. While this has been shown to produce desirable sensing outcomes in some cases, it presents a number of seemingly unaddressed problems when applied to a TICI. These include vulnerability to fibrosis [3], reliance on adequate fluid flow through the device that would be compromised by the relatively common translocation between scalae of cochlear implants during implantation or tip fold-over [4], as well as inconsistent frequency response across the device's large bandwidth (200-8,000 Hz) when only 4 to 22 individual micro-oscillators are employed.

The current work proposes to make known a subset of engineering problems beyond purely improving acoustic performance parameters, as these problems can have a detrimental effect on proposed solutions.

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P2.071 Heterogeneous Nature of Carbon Felt Investigated by Single Fibres and Intact Electrodes to Highlight Performance Variations

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Vanadium redox flow batteries (VRFBs) are a promising solution to the demand for large-scale energy storage [1]. The reactivity of VRFB electrode materials is of great interest, with previous studies on carbon felt materials revealing a significant degree of performance variability for both pristine and treated electrode samples [2-4]. Thus, the heterogeneous nature of carbon felt needs to be further investigated to better understand performance variations in VRFB systems.

In this work, a rate constant distribution has been observed for single fibre electrodes extracted from polyacrylonitrile-based carbon felt for the ferri/ferrocyanide redox reaction. Importantly, it was found that the distribution of rate constants from single fibre measurements was statistically different depending on which the side of the felt these fibres were extracted from. For this reason, the influence of intact electrode configuration on overpotential was investigated for the same carbon felt sample using the positive vanadium redox reaction. Electrochemical testing and material characterisation showed significant differences across the two electrode faces.

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P2.072 Electroreduction of NO3- to N2 on Pt(111) and Pd(111) Surfaces

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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, predominately producing NH_4+ and N_2O, with little to no N_2 produced [3].

In this work, using statistical modelling techniques we aim to rationalise the different behaviour of the Pt(111) and Pd(111) surfaces with a focus on how hydrogen coverage affects the selectivity of the reaction [4]. This stems from preliminary work in our group which found hydrogen atoms to adsorb differently to Pt(111) and Pd(111). Thus, it is hypothesised that on the Pt(111) surface hydrogen atoms are blocking the active surface sites which are required for the formation of N_2. This project extends on these preliminary results to further understand the nitrate reduction process with explicit consideration of competing processes such as hydrogen adsorption. Here it is hoped that an understanding of the various competing reactions will provide an insight into the parameters which can ideally be controlled to improve the experimental selectivity.

P2.073 The development of a controlled release hydrogel-based drug delivery system to present growth factors

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Growth factors have recently been explored as therapeutic agents for tissue engineering (1, 2). Neurotrophic growth factors (NF), specifically, have been shown to support and direct the regrowth of nerve cells and have potential for the treatment of a range of disease states and injuries, including spinal cord injuries (3). However, key challenges in using NFs include their short half-life in vivo and the potential for off-target effects (4).

These challenges could be overcome by the temporal and spatial control of NFs delivery to its target site. Therefore, a delivery system that can encapsulate NFs and achieve controlled release over weeks have the potential to improve the therapeutic efficacy of NFs.
Hydrogels were prepared from gelatin methacryoyl (GelMA), poly(N-isopropylacrylamide) (pNIPAM) and poloxamers. Different loading approaches were investigated to boost the amount of drug that could be incorporated. A model drug (FITC-lysozyme) was loaded into hydrogel-based drug delivery systems and the release profile investigated.

The results show that different loading strategies did not impact drug loading into gelatin methacryoyl (GelMA) and poly(N-isopropylacrylamide) hydrogels. All hydrogel-based systems achieved controlled release over at least one week. Modifications of hydrogel concentrations, degree of functionalisation and composition are all viable approaches to modify release profiles.

In the future, these hydrogel-based delivery systems will be loaded with NFs and NFs will be released in a controlled manner to support the regrowth of nerve cells in vivo.

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P2.074 Pelletization and Sintering of New Zealand Titanomagnetite Ironsand

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Hydrogen-direct-reduction of iron ore in a vertical shaft furnace is a potential route to significantly reduce industrial CO2 emissions from the steel industry. This approach requires pelletization of iron ore fines before they can be fed to the shaft furnace. Here we report an investigation into the disc-pelletization of NZ titanomagnetite ironsand, and its subsequent sintering and hydrogen reduction behavior. A study was initially conducted on the effect of varying ironsand particle size and sintering conditions on the strength of pellets bonded with bentonite and a commercially sourced carboxymethyl-cellulose binding agent. Green pellets containing ironsand with average particle size of 65 µm exhibited optimal strength. The compressive strength of 5 mm diameter pellets after sintering in air at 1200 °C for 2 h was determined to be 976 N, which exceeded the minimum requirement. Enhanced sintered strength was attributed to the recrystallisation of titanohematite grains from oxidation of titanomagnetite, and the formation of a liquid bonding phase from the bentonite material due to interdiffusion and subsequent melting. Alternative binders were then explored to potentially lower the sintering temperature requirement. A combination of organic and inorganic binders was found to be essential, wherein carboxymethyl-cellulose binders provided strength in green pellets, whilst inorganic additives such as bentonite, calcium borate, and fine glass, promoted high sintered strength. Finally, ironsand pellets were reduced in hydrogen gas at 1100 °C in a thermogravimetric furnace. All the pellets exhibited a reduction degree of ~97%, indicating that different pellet preparation procedures had no significant effect on reducibility.

P2.075 Effect of iron implantation into piezochromic properties of cobalt molybdate films

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Transition metal molybdates A2+Mo6+(O2-)4 (A = Co, Cu, Ni, Mn, Fe) are promising materials for many applications such as piezochromic, thermochromic, catalyst, battery electrodes and supercapacitors [1-3]. Their unique properties stem from structural features where different polymorphic forms can exist depending on the co-ordination of A2+ and Mo6+ cations in the crystal structure [1]. Phase transition can be triggered by applying strain (pressure) which influences A2+ and Mo6+ co-ordination. In iron-cobalt molybdate (Co1-xFexMoO4) material, Co and Fe oxidation states play a crucial role in stabilizing α and β-phase which give them green (α-phase) or purple (β-phase) appearance [2].

We report synthesis of Co1-xFexMoO4 by low energy Fe implantation into CoMoO4 films prepared by magnetron sputtering [4]. Dynamic-TRIM calculations of 10 keV 57Fe+ with fluence 1×1016 and 2×1016 Fe/cm2 showed peak concentration of 9.6 at% and 17.1 at%, respectively at an average depth of 7.5 nm. Co1-xFexMoO4 films were annealed in oxygen atmosphere at 700 °C for 5 hrs. Rutherford backscattering spectrometry results showed slight diffusion of Fe towards interface upon annealing the films. X-ray diffraction results showed presence of β-phase evident from its purple hue appearance. Magnetic measurements showed an antiferromagnetic transition at 10 K. The results based on compositional, structural, morphological, and magnetic measurements on Fe implanted CoMoO4 films will be presented in detail at the conference.

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P2.076 Elucidating the effect of surface passivation on crystal growth and charge carrier relaxation dynamics

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Poster Session 2 + Tech Tasters Pitch Sessions, February 8, 2023, 5:35 PM - 7:30 PM

Lead-free bismuth perovskites become popular due to nontoxic nature and rich structural diversity [1-2]. Layered double perovskites have drawn attention for the photovoltaic application as an alternative for lead halide perovskite due to their benign character and other physical properties. These perovskites exhibit appreciable photothermal stability. Cs4CuSb2Cl12 (CCSC), a double perovskite of the form A4BIIB2IIIX12, was reported to have high carrier mobility, and both direct and indirect bandgaps, lying in the visible range. Though, CCSC offers facile synthesis methods, is stable to heat, light, and humidity, and has a suitable bandgap for optoelectronic applications. However, the excited state dynamics and nature of trap states of these microcrystals (MCs) are yet to be explored.

To this end, using the solution-processed method we have synthesized bare and ligand capped CCSC MCs. Our studies revealed that in the presence of surfactant the growth of the crystals is not irregular but circular in shape. Using femtosecond transient absorption spectroscopy, we studied the excited state dynamics. The relaxation pathways were studied under different excitation wavelengths, above/near/below the absorption maxima. Since trap states play a role in the charge relaxation and transfer process, we further studied the excited state dynamics and the effect of surfactants on charge carrier dynamics. This analysis shows the presence of deep trap states in the CCSC MCs which can be passivated using suitable surfactants to make it more viable for photovoltaic application.

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P2.077 PEDOT in On-Skin Wearables: Study of the Polymer Electrochemical Stability

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Poster Session 2 + Tech Tasters Pitch Sessions, February 8, 2023, 5:35 PM - 7:30 PM

Recently, there has been an increase in employing conducting polymers in wearable devices, due to their mechanical flexibility combined with electroactivity. Up to date, there have been works highlighting the integration of conducting polymers, particularly poly3,4-ethylenedioxythiophene (PEDOT) for on-skin sensors. The polymer plays a dominant role as an active material in electrochemical transducers for sensing. However, the electrochemical stability of the polymer has not been properly addressed in previous works. Hence, this study focuses on addressing the stability of conducting polymer PEDOT in electrochemical system, which tailors to on-skin applications. Different variants of doped PEDOT, like PEDOT:tosylate (TOS), PEDOT:polystyrenesulfonate (PSS) and a new variant of PEDOT co-doped with both TOS and PSS are explored in simulated biological fluid made up of artificial interstitial fluid (aISF). The stability of the polymers is tested via two set of experiments, (1) stress test via 10,000 cyclic voltammetry (CV) cycles and (2) exposure test via immersion in aISF for two weeks. The electro impedance spectroscopy (EIS) performance before and after each tests are observed to validate the polymer's stability. Next, skin lysates are added in the aISF to imitate on-skin sensing conditions for demonstrating polymer stability towards on-skin wearables.

P2.078 Correlation of optical and structural properties of silver nanorods

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Poster Session 2 + Tech Tasters Pitch Sessions, February 8, 2023, 5:35 PM - 7:30 PM

Plasmonic silver nanoparticles offer a highly tunable platform for modulating the optical properties of nearby chromophores. To understand the detailed mechanism of chromophore-nanoparticle interactions the silver particles must have well-controlled and narrowly distributed morphologies. In this poster, I describe an optimised silver nanorod synthesis and purification procedure that can produce particles with low size and shape distributions. These particles' optical absorbance and scattering properties can be tuned across the visible to near IR spectral window. This research also describes an effective method for the fabrication of monolayer nanorod films for controllable interaction with overlayered chromophore molecules or quantum dots. Focus has been placed on controlling particle proximity during fabrication to modulate the electric field interactions between particles. These films will ultimately be used to investigate plasmon-enhanced up-conversion in polycyclic aromatic hydrocarbons.

P2.079 Transport spectroscopy and the search for Majorana zero modes

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Poster Session 2 + Tech Tasters Pitch Sessions, February 8, 2023, 5:35 PM - 7:30 PM

Semiconductor nanowire-superconductor hybrid systems provide a promising platform for hosting Majorana zero modes. However, the conclusive experimental detection is a much debated and contentious issue.

This talk plans to address the issue of whether a conductance gap closure can be used as a smoking gun for the detection of topological edge modes [1,2].

We will describe the conductance spectroscopy measurements, the topological gap protocol [2] and the current experimental status focusing especially on the “false positives” associated with this technique. Starting from the basics of quantum transport theory, we will then demonstrate how to adapt the Keldysh non-equilibrium Green’s function (NEGF) technique to understand the local and non-local conductance spectroscopy and the purported gap closure signatures [1].

Moving on, we will describe the non-locality of true Majorana modes (and topological edge modes in general) can be described via the concept of topological entanglement entropy [1] and can indeed signal a genuine transition, regardless of the constituent non-idealities in an experimental situation. Finally, we will touch upon how to extend our transport formulation to more realistic device structures [3-5] including the currently pursued magnetic insulator- nanowire hybrid set up [5], and how to include disorder and dephasing in topological devices in general [6].

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P2.080 Understanding vanadium redox flow batteries and their reactions to improve performance

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Poster Session 2 + Tech Tasters Pitch Sessions, February 8, 2023, 5:35 PM - 7:30 PM

Clean, renewable energy sources are essential for mitigating climate change [1]. However, to facilitate the use of these renewable sources, which have temporal and intermittent energy supply, energy must be stored and released to the grid during times of peak use. Vanadium redox flow batteries (VRFBs) are one promising solution to energy storage as they display quick response times, long lifespans, and can almost completely discharge [2]. Unfortunately, VRFBs are not commercially viable due to slow reaction rates at the catalytic electrode surfaces. Hence, VRFBs have yet to be widely adopted.

Catalytic activity in VRFBs may be enhanced by developing a greater understanding of the redox mechanisms of the vanadium species and their interactions at the electrode surface. While a small number of studies have found means to improve catalytic activity of VFRBs, through electrode surface functionalisation and modification of the electrolytes, very little is known regarding how these changes influence and modify the redox mechanism of the vanadium species [3]. Consequently, there is limited guidance to help aid future VFRB development. Accordingly, this work utilises computational methods, including molecular dynamics and density functional theory, to provide insight into the reactions within VRFBs that were previously unknown.

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P2.082 Adsorption and plasmonic photocatalysis in an Au-CeO2 nanosystem work in concert: experimental confirmation and plasmonic modeling

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Adsorption and plasmonic photocatalysis in an Au-CeO2 nanosystem work in concert: experimental confirmation and plasmonic modelling
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Adsorbents are secondary pollutants in the environment that are created by adsorption-mediated water treatment. Conversely, photocatalysis aids in the pollutant's disintegration into its harmless forms. Here, we show how adsorption and photocatalysis operate together in Au-CeO2 nanocomposites to completely remove methylene blue (MB) from water. Au-CeO2 with various Au loadings was synthesized using a citrate modification technique. A kinetics and thermodynamic model is used to examine its adsorption capability. We note that Ce3+ states in CeO2 and citrate ligands on Au NPs play a major role in the high adsorption capability of AuCeO2. The supported Au NPs receive electrons from the Ce3+ states by interaction, which gives Au a negative charge. The total removal of MB is expedited under white light and lasers. A control experiment with Au NPs shows less adsorption−photocatalysis. The size of Au NPs and Au−CeO2 interfacial interaction is responsible for the surface plasmon resonance spectral position at 550−600 nm. Linear sweep voltammetry (LSV) and plasmonic field simulation show surface plasmon-driven photocatalysis in Au−CeO2. LSV shows a 3-fold higher photocurrent density in Au− CeO2 than colloidal Au NPs under white light. The simulated electric field intensity in Au−CeO2 is maximum at SPR excitation and the closest interfacial separation (d = 0 nm). Notably, near-field light concentration, hot electrons, and interfacial charge separation are responsible for excellent MB removal in the Au−CeO2 nanosystem.

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P2.083 Electrospun magnetic (Ni1-xFex, MnFe2O4, and MnSmxFe2-xO4) nanofibers for potential flux-guiding applications

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Magnetic nanofibers possess thin dimensions, large surface areas, and a high magnetization [1]. Their high shape anisotropy and uniaxial directions can be useful in flux guidance and in the reduction of eddy-current losses. Ni1-xFex and MnFe2O4 are the most favorable soft magnetic materials in flux guiding applications for inductive power transfer systems. The fabrication of polymer nanofibers containing Ni1-xFex and MnFe2O4 nanoparticles can help in the reduction of eddy-current losses and can be further advantageous as the small size can lead to superparamagnetism [2]. Doping of MnFe2O4, a well-known commercial ferrite, can enhance the magnetic properties [3]. Despite the potential advantages of magnetic nanofibers, there have been very few studies focusing on Ni1-xFex, MnFe2O4, and doped MnFe2O4.
In this study, we report the fabrication of polymer nanofibers containing Ni1-xFex (x=0.1-0.5), MnFe2O4, and Sm3+ doped MnSmxFe2-xO4 (x=0.06-0.25) made by the electrospinning method. These nanofibers have a quasi-uniaxial direction and interesting growth mechanisms. The Ni1-xFex nanofibres all contained nanoparticles where the x~0.5 nanoparticles were superparamagnetic. Magnetic nanoparticles and single crystalline nanorods were observed for the MnFe2O4 nanofibers with a high saturation magnetization. Sm3+ ions were successfully incorporated into the crystal structure of MnFe2O4 where the Sm-doped nanoparticles resulted in a decrease in the nanoparticle size and the appearance of superparamagnetism at high Sm fractions. This work has laid a solid foundation for future investigations of soft magnetic nanofibers preparation methods and subsequent applications.

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P2.084 Investigation of mechanical cell compression and recovery at the microscale

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Mechanical forces shape physiological structure and function within cell and tissue microenvironments. When exposed to forces, cells strive to restore their shape or develop an adaptive mechanism to maintain cell integrity depending on strength and type of the mechanical loading [1]. With the purpose of applying mechanical compression in a cyclic, dynamic and controlled manner for the investigation of cell deformation and recovery at microscale, we have recently developed a robust cyclic compression microfluidic method based on a flexible microdevice [2]. In this work, we extend the use of the platform to the application of sequential cyclic compressions at and beyond physiological pressures to study dynamic biomechanical processes by recording GFP-tagged actin dynamics of live cells under compression. Using time-lapse imaging, we thus show a sequence of actin deformation and disruption events based on the amount of the applied pressure. We further showcase data of cellular deformations and recovery during and after cyclic compression at mild (~15.6 kPa) and upper mild (~20.8 kPa) physiological pressures, obtained via end point assays of actin and nuclei deformations at zero time or at 24 h-recovery after compression. Differences observed between compressed cells fixed at zero time or after 24 h-recovery suggest that SKOV-3 cells exhibit deformations at the time of applied compression, a proposed mechanism cells use to prevent mechanical damage. As demonstrated in this work, the extent of recovery of compressed cells can give insights into the mechanics of cancer cells when exposed to various levels of compressive stress applied at microscale.

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P2.085 Modification of superconductivity in lead through the use of embedded nanoparticles

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Poster Session 2 + Tech Tasters Pitch Sessions, February 8, 2023, 5:35 PM - 7:30 PM

Superconducting films of Pb were altered through ion implantation with the aim of inducing string in the surface and taking advantage of the superconducting pressure effect in Pb. Ions of Ni were used to induce positive pressure, Si for negative pressure and Pb to show the effect of disorder. An acceleration voltage of 20KeV was used to deposit the ions in the surface of the films. The concentration was varied buy adjusting the duration of implantation.

Magnetisation curves taken in a squid show the transition temperature shift by [~1.5K] which is roughly equivalent to [~1Gpa] of pressure when applied externally. Pb in Pb samples show no shift in Tc demonstrating that the effect is not due to defects in the Pb films but from the implanted ions themselves. TEM scans show the internal structure and the formation of nanoparticles within the surface of the thin films. Along with RBS scans this verifies the composition of the films and distribution of the ions in the surface.

P2.086 Tracking Exciton Diffusion in Framework Materials via Ultrafast Transient Absorption Spectroscopy

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Measuring the exciton diffusion properties of framework materials is under increasing interest due to its potential in real-world applications such as photo-induced catalysis and light-harvesting. The optimization of exciton diffusion lengths and lifetimes has been furtherly researched using a variety of framework materials such as covalent organic frameworks (COFs) and metal-organic frameworks (MOFs), but little research has been done to investigate how the exact chemical and physical structure of these framework materials directly impacts its exciton diffusion properties. Here, we investigate how the chemical structure of framework materials impacts their exciton diffusion properties using ultrafast spectroscopic techniques to measure the ultrafast dynamics involved in exciton diffusion. The framework materials used in this project were provided in collaboration with other groups and will be used in the creation of a library, with each material containing slight variations in chemical structure. This library allows for the systematic measuring of exciton diffusion properties in relation to chemical structure. We start by investigating a series of MOFs made up of truxene derivative linker molecules and Zn metal nodes, along with the creation of crystal particle dispersion that can be studied by ultrafast optical spectroscopy.

P2.087 Exploring the Selectivity of Copper-catalysed Phosphoramidate Synthesis in Ionic Liquids

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Traditionally phosphoramidates have been synthesized by the nucleophilic substitution of chlorophosphonates with amides in the presence of a strong base such as n-butyllithium.[1] Recent methods involve aerobic oxidative dehydrocoupling, where phosphites interact with a copper(II) bromide catalyst to produce a halogenated phosphite and copper(I) bromide.[2] The reduced copper(I) is re-oxidized by air, thus completing a catalytic cycle. The aerobic oxidative dehydrocoupling reaction was examined using ionic liquids as alternative solvents in an effort to explore their kinetic and thermodynamic effects on the reaction. Conditions were also explored using different copper catalysts, as studies in literature have indicated an anion effect on the aerobic oxidation of amines where selectivity between imine and nitrile product could be controlled.[3] $[C_4C_1im][Me_2PO_4]$, $[C_4C_1im][OAc]$, and $[C_4C_1im][NTf_2]$ were used as ionic liquid solvents and compared to ethyl acetate (EtOAc), the most commonly used solvent for this transformation. Copper catalysts included $CuBr_2$, $Cu(OAc)_2$, $CuCl_2$, and $Cu(OTf)_2$. This presentation will outline the effect of the aforementioned ionic liquids and copper catalysts on the selectivity of phosphoramidate and imine products discussing the effects and mechanisms underlying the changes observed.

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P2.088 Assessing interfacial strength of CF/thermoplastic composites after continuous air plasma jet fibre treatment

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Fibre-reinforced recycled-thermoplastic composite is a material class which can assist in the reduction of future environmental harm if their manufacture becomes economically feasible. Inferior interfacial bonding between carbon fibre (CF) and thermoplastics compared to non-recyclable thermosetting matrix systems is a fundamental drawback [1]. Polymer recycling challenges further discourage the production of high-performance composites from waste thermoplastics.

There has been considerable effort in improving interfacial properties between CF and thermoplastics including: polyamide-12 [1], polyimide [2], polypropylene [3], or poly(ether-ether-ketone) [4] by plasma treatment. These studies are usually limited to un-sized or sized for epoxy [3] CF, test a single thermoplastic matrix and use diverse plasma sources. Additionally, there is composite manufacturing variability for interlaminar shear strength testing or single fibre fragmentation testing. As a result, the effects of plasma parameters are usually not comparable between papers for a specific CF/matrix combination.
In this work, we build on previous studies by incorporating differently sized as-received CFs in a continuous, non-equilibrium, atmospheric-pressure, air plasma jet treatment process. SEM, FT-IR and XPS will characterise morphological and chemical modification. Compression moulded specimen short-beam strength will be tested to assess fibre-matrix bonding.

The techniques above will be used to optimise the fibre-plasma nozzle distance for a single CF/polymer combination. We hypothesise that the optimal plasma treatment time on the same experimental setup will differ between CF/polymer combinations due to varying fibre coating and polymer surface energy. Presented results will identify which recyclable polymers are compatible with high process-speed and high-performance plasma-treated CF for thermoplastic tape manufacture.

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P2.125 Interfacial colloidal assembly guided by optical tweezers and tuned via surface charge.

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The size, shape, and dynamics of assemblies of colloidal particles optically-trapped at an air–water interface can be tuned by controlling the optical potential, particle concentration, surface charge density and wettability of the particles and the surface tension of the solution.
The assembly dynamics of different colloidal particle types (silica, polystyrene and carboxyl coated polystyrene particles) at an air–water interface in an optical potential were systematically explored allowing the effect of surface charge on assembly dynamics to be investigated. Additionally, the pH of the solutions were varied in order to modulate surface charge in a controllable fashion. The effect of surface tension on these assemblies was also explored by reducing the surface tension of the supporting solution by mixing ethanol with water.

Silica, polystyrene and carboxyl coated polystyrene particles showed distinct assembly behaviours at the air–water interface that could be rationalised taking into account changes in surface charge (which in addition to being different between the particles could be modified systematically by changing the solution pH). Additionally, this is the first report showing that wettability of the colloidal particles and the surface tension of the solution are critical in determining the resulting assembly at the solution surface.

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P2.089 Antimicrobial peptide-conjugated nanoparticles against bacterial pathogens

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Antibiotic resistance against multidrug-resistant (MDR) pathogens is a rising global health concern. Antimicrobial peptides (AMPs) (Zhang and Gallo, 2016) are one of the leading candidates to combat MDR pathogens due to their selective interaction with the bacterial membrane. However, AMPs have poor enzymatic stability and low permeability across biological barriers, which hinders their therapeutic development. Conjugation of antimicrobial peptides to high surface area spherical-shaped gold nanoparticles (AuNPs) to improve the antibacterial activity as well as enhance enzymatic stability and bioavailability has been undertaken (Rajchakit and Sarojini, 2017). We report on the design, synthesis, and antimicrobial analysis of potent AMP-conjugated AuNPs with negligible cytotoxicity.

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P2.090 Incorporation of Switchable Inorganic Building Blocks into Heterometallic Coordination Polymers

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Transition metal complexes of terpyridine-based ligands have aroused considerable interest within the broad field of coordination chemistry due to their interesting magnetic, electrochemical, photophysical and catalytic properties.1-3 Terpyridine-based ligands have found a particular use in supramolecular assemblies due to the ease of modifying substituents at the 4-position of the terpyridine ring, allowing for the addition of secondary binding units 'out the back' of the terpyridine moiety.4 Cobalt complexes of terpyridine, of the type [Co(tpy)2]2+ are well known to undergo a spin transition (spin crossover) from the low spin (S = 1/2) to high spin (S = 3/2) state upon thermal stimuli,2 opening them up for use as molecular switches.

Herein we report the synthesis of a new asymmetric ditopic 1,2,4-triazole-terpyridine ligand (Ltpypyr). Monometallic [MII(Ltpypyr)2]2+ (MII = FeII, CoII, RuII) complexes are reported and fully characterised including magnetic, and electrochemical measurements. All three complexes show reversible MII/IIIoxidation processes while [CoII(Ltpypyr)2]2+ also shows spin crossover behaviour in the solid state. We show that it is possible to link these units into 1D and 2D heterometallic polymers using CuI and AgI metal ions. The spin crossover activity of [Co(Ltpypyr)2]2+ is conserved when the unit is incorporated into the larger architecture.

P2.091 Electrochemical Synthesis of Ammonia Based on Transition Metal Nitrides

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Electrocatalytic Nitrogen Reduction Reaction (ENRR) is a viable method for decarbonising the ammonia (NH_3) fertiliser industry while also serving as a hydrogen energy carrier[1]. Several key challenges highlighted in ENRR includes strong nitrogen activation, poor nitrogen solubility, breaking scaling relations and low NRR selectivity contribute to extremely low NH_3 yield and Faradaic efficiency. The Mars-van Krevelen (MvK) mechanism has a unique advantage in NRR when the surface layer containing N is electrochemically reduced to NH_3 and the resulting vacancy is replenished with N_2 to regenerate the catalyst. Among other catalysts explored, the fact that transition metal nitrides (TMNs) follows this mechanism makes it even more promising[2].

For this conference, we present our recent progress on the development of thin film TMNs electrocatalysts for NRR via nitrogen ion implantation on metal. The amount of implanted nitrogen $^{14}N+$ are adjusted during ion beam with an acceleration energy of 10 keV at dosage of 0.9 to 3.0 × 10^{17} at/cm^2. The elemental composition and variation in film thickness with respect to nitrogen implantation are analysed with RBS and NRA studies[3]. The crystalline properties are investigated with XRD and topographical properties with AFM. Then, the electrical properties are measured with the Hall probe setup. The electrochemical performance of the prepared catalysts is also compared in an Ar-saturated and N_2-saturated chamber under ambient conditions. This research is expected to shed light on the challenges of designing NRR electrocatalysts with high selectivity towards ammonia production, as well as the chosen strategy for overcoming practical difficulties in this field.

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P2.092 Rust fungi culture on artificial flat and heterogenous surfaces – A key stepping stone to Lab-on-a-Chip devices

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Exacerbated by a changing climate, New Zealand faces growing risks from the impacts of plant diseases. Many of NZ's highly-valued native trees - mānuka, pōhutukawa, rātā - are currently under threat by the fungal disease myrtle rust (MR), caused by the obligate biotrophic fungus Austropuccinia psidii [1]. MR has never been eradicated from any country and thus requires novel tools to help with impact mitigation and long-term management. In particular, there is an urgent need to screen large numbers of biological control agents (BCA) for their ability to reduce A. psidii's virulence. Lab-on-a-chip (LOC) devices can accelerate such screening by enabling pathogen-BCA interactions to be observed at a single-cell level with high-throughput [2]. One problem with these devices is that they require the pathogen to be grown separately from its natural host(s) in an artificial environment. Since MR requires a living host to complete its asexual reproductive life cycle, growth on artificial surfaces is currently seen as impossible. Using wheat leaf and poplar rusts as model species, we report on recent successes in the growth of rust fungi on artificial substrates. These substrates include flat and heterogeneous high-resolution leaf surface replicates made of either silicone polymers [3] or agar-based media. We show preparation of the substrates and observed growth in the absence of host plants. The latter consisted of surface growth, surface penetration and internal growth within the artificial substrates. Based on these results, existing LOC devices [4] are now being modified to host rust fungi for BCA screening applications.

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P2.093 Electrochemically Grafting of Aryldiazonium Films onto Perovskite Surfaces to Act as Charge Extraction Layers

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Metal halide perovskites continue to be at the center of solar cell research due to their excellent absorption coefficient, tunable bandgap, long charge carrier diffusion lengths and they are relatively simple to fabricate.[1] The problem with perovskites is that they have no mechanism to separate the photo-generated charges, and therefore require additional charge transport layers to be deposited on either side of the perovskite absorber.[2] These materials limit the performance of a solar device because they are only mechanically bound, reduce the light intensity reaching the absorber, and require surface engineering to align the band-edges to facilitate charge transfer.[3] Our aim is to replace the charge transport layers with thin organic films containing functionality that aids the charge extraction whilst minimizing optical losses. We are doing this by electrochemically grafting thin films to perovskite surfaces using the well-known reduction of aryldiazonium ions in solution.[4] This method of modifying the perovskite interface is unexplored and provides a new avenue for controllable engineering of perovskite solar cells.
The aryldiazonium grafted thin films were investigated using voltammetry, electrochemical impedance spectroscopy, UV-visible and photoluminescence spectroscopies, XPS, and imaged using SEM and AFM. Presented are the results of these studies.

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P2.094 Atypical vesicles and membranes with monolayer and multilayer structures formed by graft copolymers with diblock side-chains

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Graft copolymers with diblock side-chains Am(-graft-B3Ay)n in a selective solvent have been reported to self-assemble into vesicles, but the structure is expected to differ distinctly from lipid bilayers. Surprisingly, the number of the alternating hydrophobic A-block and hydrophilic B-block layers in the vesicle can vary from monolayer to multilayer such as hepta-layer, subject to the same copolymer concentration. The area density of the copolymer layer is not uniform across the membrane. This structural difference among different layers is attributed to the neighboring environment and the curvature of the layer. Because of the unusual polymer conformations, nonlamellar structures of polymersomes are formed, and they are much more intricate than those of liposomes. In fact, a copolymer can contribute to a single or two hydrophilic layers, and it can participate up to three hydrophobic layers. The influences of the backbone length (m) and side-chain length (y) and the permeation dynamics are also studied. The thickness of hydrophobic layers is found to rise with increasing the side-chain length but is not sensitive to the backbone length. Although the permeation time grows with the layer number for planar membranes, the opposite behavior is observed for spherical vesicles owing to the curvature-enhanced permeability associated with Laplace pressure.

P2.095 All-Gel Sensor based Wearable Device for measuring blood pressure

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Although interest in healthcare and remote diagnosis is being continuously increased, conventional electrodes and sensors used in measuring biosignals are not suitable in new remote medical systems due to lack of convenience and portability. Especially, conventional products based on hydrogels, which are commonly used to measure blood pressure (BP) and electrocardiogram (ECG), rapidly deteriorate its performance over time. In this study, wearable, all-gel-based sensors to simultaneously acquire the pulsation and ECG without cuff at single site were developed. Poly (vinylidene fluoride-trifluoroethylene) gel and polyvinyl chloride ion gel were used for the pulsation and ECG measurement, respectively. A combined gel sensor with stretchability and flexibility was fabricated and easily attached to the wrist, where radial artery is located. Then, pulsation and ECG were successfully measured at one point simultaneously even after 30 days. After calculating the phase time difference between two signals, the algorithm for BP calculation was demonstrated.

P2.096 Luminescence and electron trapping properties of isoelectronic Ln3+/Ln2+ ions in fluoroperovskites

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As digital information is produced at an ever-increasing rate, new data storage technologies with increased capacities, longer lifetimes, and faster read/write speeds must be developed[1]. Optical storage media require less energy to operate than conventional electronic and magnetic media and have potential storage lifetimes exceeding 100 years. However, these media are typically limited by low storage capacities. Consequently, it is of interest to investigate novel materials that can store data via luminescence, and methods by which high storage capacities and long storage lifetimes can be achieved.

We present the results of studies on the luminescent fluoroperovskite compounds NaMgF3:Ln (Ln = Ce, Pr, Nd, Sm, Eu, Tb, Dy, Ho, Er, Tm, or Yb). We show that Ln dopants substitute into the host lattice and produce characteristic luminescence. Several compounds exhibit mixed-valence behaviour (Ln2+/Ln3+), where the concentration of divalent Ln depends on the location of the 4fn ground state relative to the conduction band of the host[2]. The concentrations of each valence can be further controlled by inducing electron-trapping via cross-band stimulation (Ln3+ → Ln2+), and electron liberation via optical stimulation (Ln2+ → Ln3+). In some cases, the electron trap energies exceed several eV, such that the Ln2+ ions are highly stable, and the concentration can be probed optically and non-destructively[3]. Ultimately, we demonstrate that optically reversible conversions Ln3+ ↔ Ln2+ are possible in fluoroperovskite host compounds, providing a mechanism of luminescent data storage, and that long lifetimes and high storage capacities are achievable.

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P2.099 A New Family of Group 14 Aluminium Bimetallic Complexes

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We have developed a new series of heterobimetallic Group 14 – aluminium complexes using the low valent aluminyl compound [(NONDipp)AlK)] (NONDipp = [O(SiMe2NDipp)2]2- , Dipp = 2,6-iPr2C6H3][1], including the first example of a Pb-Al bond. This poster will examine the synthesis and reactivity of this new family of bimetallic complexes, [(NONDipp)Al-M(AMIDipp), (AMIDipp = [C(tBu)(NDipp)(NHDipp)], M = Ge, Sn, Pb). Their solid-state structure and solution phase behaviour will be examined. These Al-M heterobimetallics activate alkynes, resulting in the insertion of alkynes into the Al-M bond. For example, phenyl acetylene inserted into the Al-Ge bond to form [PhC_2H(Al{NONDipp})(Ge{AMIDipp})]. Comparisons with other main group bimetallic systems will also be discussed.[2,3]

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P2.100 Use of structure and memory for the global optimisation of atomic clusters

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Clusters are collections of atoms that form nanoscale particles. Metallic clusters are of particular interest as they exhibit properties unique from the bulk, lending them to applications such as catalysis, sensors and imaging. The specific properties of a cluster depend on its structure, thus structural determination is a crucial step for identifying clusters for use in a given application.[1]

Global optimisation (GO) algorithms are used to search for the lowest energy structure – or global minimum – of a cluster, by exploring its potential energy surface (PES). Unfortunately, even small clusters have very large PESs, making it prohibitive to check every possible isomer. Instead, GO algorithms typically identify and sample low energy region(s) of the PES. However, when two or more such regions exist on a PES, the algorithm often struggles to explore them all, instead becoming trapped in a single region.[2]

The basin-hopping algorithm, an example of a GO algorithm, takes a starting structure and perturbs it randomly to locate a new, related structure. The 'hop' to this new structure is accepted or rejected based on the change in energy, after which this process repeats many times.[2] This project has augmented the algorithm to also consider structure and memory on top of energy, to encourage the exploration of multiple low energy regions. This presentation will detail these methods and their effect on algorithmic efficiency. It is hoped these methods can also be applied to an ongoing study of copper clusters being screened as candidates for CO_2 reduction catalysts.

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P2.101 Complexity Analysis of Physical Percolating Nanoparticle Networks

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Percolating nanoparticle networks (PNNs) offer a potential pathway towards a future, neuromorphic, computing architectural design. These networks exhibit many desirable properties of neuromorphic systems, for example: low power, low cost, and readily scalable. Furthermore, at the percolation threshold, the networks self-organise into a critical state which has been hypothesised as a necessity for optimum computational ability to occur [1]. It has been previously shown that PNNs share many of the same emergent phenomena as the mammalian brain, including long-range temporal correlations, scale-invariant properties, and critical avalanche dynamics [2]. Here, we present both a qualitative and quantitative analysis of the inherit complex dynamics observed from multiple simultaneous readouts of a PNN. Several qualitative measures of complexity are developed and explored, as well as the quantitative metric of Neural Complexity [3] that has previously been applied to biological neuron systems [4].

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P2.102 The Role of Optimized Parameters for Simple Geometries in the Production of Complex Architectures

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The purpose of this study is to determine the optimal 3D bioprinting parameters for shape accuracy utilising basic geometries on a Biobot Basic bioprinter from Advanced Systems to later fabricate complex organ-like tissues. In order to compare and optimise bioprinting parameters, Pluronic F-127, a shear thinning hydrogel, was used to print cubes, cylinders, and square pyramids. For bioprinters, official measures of printability and shape fidelity are still in early development[1], with little research done into prints consisting of more than 2-3 layers[2]. Pluronic-F127 is a common hydrogel used in bioprinting for simulating human tissue that has consistent reports of high printability and was thus chosen for this research[3]. To assess shape fidelity, measurements of height, width, diameter, surface area and wall angle were taken from a set of 81 printed samples. The measured values were compared to what the ideal dimensions should have been to determine the effect of each varied bioprinter parameter on shape fidelity. The printing parameters investigated were printing pressure, printing-head speed and line height. Design of Experiments and statistical analysis will be applied to the results to find the optimal parameters to produce each shape. After which, the optimised printing parameters for simple geometries will be applied to more complex architectures and tissues, such as 3D prints of the liver, heart and trachea. We hypothesise that printing with optimised parameters will improve shape fidelity when compared to pre-optimised parameters. This research will inform future development of optimised 3D bioprinting parameters and fabrication of complex organ-like geometries.

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P2.103 Computing using spiking behaviour of percolating networks of nanoparticles

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Percolating networks of nanoparticles (PNNs) exhibit brain-like properties such as long-range spatiotemporal correlations and critical dynamics [1]. For this reason, PNNs are candidate systems for neuromorphic computing. Previous work has demonstrated the information processing capability of PNNs in a reservoir computing framework. Tasks such as waveform discrimination and chaotic time series forecasting were performed with the PNNs operating in a low voltage tunnelling regime [2]. Spiking occurs when higher voltages are applied, causing the formation and destruction of atomic scale filaments [3]. This work aims to exploit spiking behaviour of the PNNs to perform computation by encoding information in the timing and position of spiking events. Initial results show statistical differences in spiking activity for different input signals, and simple binary patterns have been classified using leaky integrate-and-fire neurons implemented in software. To classify more complex inputs, brain inspired learning models such as spike timing dependent plasticity and lateral inhibition will be investigated.

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P2.104 Gelatin-Based Water-Soluble Conductors for Transient Electronics

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Transient or biodegradable electronics is an emerging class of electronics, which could be completely or partly disintegrated into environment-friendly by-products after a stable operation with the programmable lifetime. Previous studies have focused on inorganic materials, mainly active metals, which is imbedded into the degradable or dissoluble matrices to achieve the degradable property. However, conducting polymers-based transient electronics have rarely been reported. In our project, we fabricated a new class of water-soluble transient electronics by attaching organic conducting polymer (poly(3-hexylthiophene), P3HT) to a biopolymer (gelatin) via the covalent bond. Sufficiently long-conjugated conducting polymers could be guided into the space between gelatin and form crystalline domains within the amorphous domains of gelatin. The biopolymer backbone is expected to facilitate the whole composite to break down under physiological conditions, where the conducting polymers parts would be enfolded by the hydrophilic shell of gelatine chains and the final micelle-like particle will be generated to help metabolize from the body.

P2.106 Tribovoltaic effects on metal-TiO2 heterojunction interfaces for mechanical-to-electrical energy conversion

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Tribovoltaic (TV) devices has been reported in 2018 as an alternative approach for mechanical-to-electrical energy conversion [1]. TV devices are made from solid semiconductors-semiconductor or metal-semiconductor sliding heterojunctions. On sliding, the friction causes the electronic excitations and heating. The induced charges are separated by the built-in electric field and transmitted over the junction or travel away from hot interface due to thermoelectric effect [2]. Other mechanism for current generation in TV device is the separation of depletion region at the p-n or Schottky junction [3].

The benefit of TV devices is high power density and continuous DC generation. DC densities up to 1x108 A m-2 has been reported [4]. For comparison, piezoelectric and triboelectric nanogenerators produce AC up to 0.1-1 A m-2.

So far, different heterojunctions have been tested for TV devices. However, there is ample of room for further improvements. No exact rules have been set to identify best sliding heterostructures.
We report tribovoltaic effects on metal-TiO2 sliding junctions. The TiO2 films were deposited by reactive DC magnetron sputtering. Microscale contact devices shown two times larger DC output than microscale metal-semiconductor junctions reported so far [5]. We chosen the TiO2 due to its good charge transport properties. DC output was investigated for six metals having different work functions. The highest charge density 1.44 mC m-2 was achieved for anatase-Mo. Amorphous TiO2 shown as two times lower DC output. Electric measurements indicate the electron transfer from metal to TiO2, thus the working mechanism is hot electron transfer or thermoelectric effect.

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P2.107 Exploring the detection of nanoplastics through the spatial interactions of gold nanoparticles in a gold-polystyrene SERS system.

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Plastic is one of the most ubiquitous forms of emerging contaminants affecting the global environment. Whilst invisible to the naked eye, nanoplastics in particular exhibit many ecological and biological implications that are not well understood. With increasing awareness of the toxicological implications and the transboundary nature of the plastic problem, the ability to detect nanoplastics for regulatory purposes is of vital importance. (1)

Surface-enhanced Raman spectroscopy (SERS) is a proven way to detect dilute analytes and has recently gained traction to detect nanoplastics in the environment. In SERS, metallic nanostructures are optically stimulated to generate surface plasmon which enhances the Raman signal of nearby chemical species. (2) Though it is known that signal enhancement depends on various materials parameters such as composition, morphology, interparticle distancing and surface area, knowledge regarding how to optimise their interplay for nanoplastic detection remains elusive. Building upon a previously developed SERS system in which gold and analyte are drop-cast onto filter paper, (3) this study begins to further understand how the size and shape of gold contribute to the signal enhancement of polystyrene nanoparticles.

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P2.108 At last, a theory of high-Tc superconductivity?

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After 35 years since the discovery of high-Tc superconductivity in cuprates, sparking the most intense investigation in any subject in physics and the development of wide-ranging applications, a comprehensive theory has now at last been claimed [1] and then backed by a beautiful set of experiments [2]. The idea is that the same superexchange interaction that leads to magnetism in the cuprates is responsible for binding electrons into the Cooper pairs that mediate superconductivity. The basic idea has been around for a long time but the ability to solve the relevant equations has only recently been developed. Several important predictions are made that explain some long-known facts [3,4]. And then, hard on its heals, the theory was quantitatively validated by some elegant STM experiments on Bi2Sr2CaCu2O8 (Bi2212), making use of a curious feature of this particular cuprate [2]. Because of the mismatch between Bi-O and Cu-O bond lengths, Bi2212 has a superlattice distortion that involves an apical oxygen moving up and down across the wavelength of the superlattice. STM measurements were used to track this modulation and its effects on energy gaps and Cooper pair density. These effects agree beautifully with the superexchange predictions. But has this 'holy grail' of condensed matter physics really been found? What are the remaining questions? Are there possible show-stoppers? What would clinch it? This talk surveys the history, the ideas, the experiments and the questions.

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P2.109 Transport current characterisation of the magnetic field-angular dependence of the critical current density for bulk REBCO superconductors

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Computer modelling of bulk superconductors produced from rare-earth barium cuprates (REBCO) is important in the development of various applications, such as bearings, projected field magnets and levitation devices. Accurate models require input data that describes the critical current density, J_c, and flux-flow exponent, n, of the superconductor as a function of temperature, and magnetic field amplitude and orientation. However, at present there is a dearth of J_c (T,B,θ) and n(T,B,θ) data for REBCO bulks.
In this work, a technique is described to obtain such data via transport critical current measurements using the SuperCurrent instrument at the Paihau-Robinson Research Institute, which has been specifically developed to characterise the angle-, temperature- and field-dependence of critical current in HTS wires. Superconducting bars with cross-sections of less than 5 mm² were cut from Ag-infused GdBCO bulks using a diamond wire band saw, and then mounted and polished to produce measurement samples. Four-point probe measurements of transport I_c have then been performed using the SuperCurrent system, which enables measurements at a range of temperatures (down to ~15 K), and with applied fields of up to 8 T and over 360 degrees orientation. Preliminary measurements of REBCO bulks made using this method are reported, in particular, the highly anisotropic field dependence observed, in addition to significant temperature dependence of both self-field I_c and n-value.

P2.110 Sulfur copolymers for thermal imaging and clandestine surveillance

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With increasing use of infrared imaging in medical diagnostics, military and civilian surveillance, and navigation of autonomous vehicles, there is a need for low-cost alternatives to traditional materials used in infrared optics such as germanium. Sulfur-rich copolymers hold promise, as they are made from low-cost feedstocks and have a high refractive index. In this report, cyclopentadiene was copolymerized with sulfur to provide a plastic with the highest long-wave infrared transparency reported to date for this class of materials. Diverse lens architectures were accessible through melt casting or injection molding. The featured copolymer was black, which enabled its use as an infrared-transparent blind for protection of thermal imaging equipment and clandestine surveillance. These findings portend to expanded use of sulfur copolymers in infrared optics.

P2.111 Structural Models of Carbon Nanomembranes

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Carbon nanomembranes (CNMs) are thin-film materials with promising applications in particle separation technologies [1]. With thicknesses of order 1 nm, CNMs are synthesised from self-assembled monolayers of aromatic or aliphatic precursors. Electron bombardment under vacuum drives off the hydrogen, creating a mechanically robust cross-linked carbon structure with a reproducible distribution of sub-nanometre-sized holes [2,3]. The hole size facilitates the rapid and selective transport of water which is thought to proceed via a cooperative single-file mechanism [3,4]. This combination of permeance and selectivity makes CNMs attractive for water purification.

Here, molecular dynamics simulation is employed to determine the atomic microstructure of CNMs. Buldge test impose sharp constraints on the Young's modulus, suggesting the network has minimal graphenic nature. Data from charged-ion spectroscopy (CIS) further constrains the interplay between holes and thickness. Our simulations explore the carbon structure within these bounds, with the ultimate goal being realistic simulation of water transport.

The carbon EDIP potential is used to perform annealing simulations from random carbon-only initial configurations with precursor thickness and density the only parameters. Pre-determined hole patterns are enforced using an in-house code; these are tuned against simulated CIS spectra and experimental Atomic Force Microscopy data. Difficulties in reconciling the predicted and experimental data sets suggests that air stabilisation (in particular, chemical reactions with moisture) is a crucial aspect of the CNM, a factor which is seldom discussed in the literature.

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P2.112 Thermally assisted mobility of nanodroplets on surfaces with weak defects

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Thermal activation plays an essential role in contact line dynamics on nanorough surfaces. However, the relation between the aforementioned concept and the sliding motion of nanodroplets remains unclear. As a result, thermally assisted motion of nanodroplets on nanorough surfaces is investigated in this work. Steady slide and random motion of nanodroplets on surfaces with weak defects are investigated by Many-body Dissipative Particle Dynamics. The surface roughness is characterized by the slip length acquired from the velocity profile associated with the flowing film. The slip length is found to decline with increasing the defect density. The linear relationship between the sliding velocity and driving force gives the mobility and reveals the absence of contact line pinning. On the basis of the Navier condition, a simple relation is derived and states that the mobility is proportional to the slip length and the reciprocal of the product of viscosity and contact area. Our simulation results agree excellently with the theoretical prediction. In the absence of external forces, a two-dimensional Brownian motion of nanodroplets is observed and its mean square displacement decreases with increasing the defect density. The diffusivity is proportional to the mobility, consistent with the Einstein relation. This consequence suggests that thermal fluctuations are able to overcome contact line pinning caused by weak defects.

P2.113 Two-photon polymerisation 3D printing and its applications

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Micro- and nanofabrication, as used for integrated circuit manufacturing, consists predominantly of a large number of repetitive 2D processing steps. Modern etching technologies have enabled what essentially are 2.5D structures, but large-area, free-form 3D patterning at the nanoscale has remained out of reach. This paradigm is now increasingly being challenged by advances in 3D printing technology, with two-photon polymerization (2PP)[1] quickly becoming the new standard for micro- and nanofabrication.[2] As opposed to stereolithography, where a UV laser scans the surface of a photosensitive material to produce a 2D pattern of polymerized material, 2PP polymerizes a material along the trace of a laser focal point moving through a resin, thus enabling fabrication of fully 3D patterns.[3] This difference in pattern generation is achieved by initiation of 2PP within the small volume of the material via precise focusing of near-infrared femtosecond laser pulses. As such, 2PP achieves higher resolution then stereolithography and is not limited to the traditional layer-by-layer approach. To make this technology available to researchers in New Zealand, the University of Canterbury Nanofabrication Laboratory recently commissioned a commercial 2PP system in form of a Nanoscribe Photonic Professional GT2 (PPGT2).[4] In this paper, we will discuss the physics behind 2PP, introduce the PPGT2 system, its operation and printing materials,[5] and showcase a selection of application examples, both in form of general micro- and nano structures,[67] as well as diffractive optical elements.

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P2.114 Vibration frequencies in rare-earth nitrides; Raman spectroscopy and DFT modelling

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The vibrational excitations in the rare-earth nitrides (as in all crystalline solids) have a defining influence on their thermal properties, but techniques for their full characterisation are substantially limited compared to those for electronic excitations. The most common study, infrared absorption spectroscopy, has yielded the frequency of only the infinite-wavelength transverse optic mode [1], no more than a single point of comparison with computed vibrational frequencies. The common second measurement, Raman scattering by phonons, is forbidden in the NaCl structure adopted by the materials. Nonetheless there is strong defect-activated scattering from the longitudinal mode [LO(L)] that has been a puzzle for a decade [2,3].

In this poster we will present a full study of inelastic Raman scattering with incident photons spanning the visible, supported by polarisation-resolved measurements in epitaxial single-crystal films. Surprisingly, there appears to be no evidence of Raman activity from nitrogen vacancies, the most common defect; rather it appears that it is grain-boundary activated. In addition to the LO(L) mode we have resolved broad scattering that is compared to the DFT-computed density of modes permitting refinement of the computational parameters. In addition to supporting the modelling procedure, the density of modes is of importance toward the development of the rare-earth nitrides as potential working materials for demagnetisation refrigeration [3].

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P2.115 Infrared study of the magnetic van der Waals Semiconductor, $Co_2P_2S_6$

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Layered van der Waals transition-metal phosphorous trichalcogenides offer the opportunity to explore a range of correlated-electron physics, such as charge density, magnetic ordering, and superconductivity, down to the 2D limit [1]. Of this class of materials, $Co_2P_2S_6$ and its doping has yet to be studied as extensively as its Fe, Ni or Mn based counterparts which have shown coupling of electronic, lattice and magnetic degrees of freedom [1,2]. Infrared spectroscopy provides a valuable perspective on such physics, but similarly to date has not been widely used to study these materials [3].

Here we report results of the first temperature-dependent optical spectroscopy studies of bulk $Co_2P_2S_6$ single crystals, from the far-infrared to the visible region of the spectrum. $Co_2P_2S_6$ transitions from a paramagnetic to antiferromagnetic state with Néel temperature T_n ~ 120 K [4], and this transition is clearly reflected through changes in the infrared spectra. At 300 K there are four relatively narrow phonon modes, a very broad mid-IR absorption and a low energy interband transition at 0.87eV. Below T_n, many modes split and the asymmetry of the lowest energy mode, which results from coupling to a low energy electronic continuum, increases. In contrast, the sample with ~20% Zn substitution of Co shows no magnetic transition, reduced asymmetry and a temperature dependence of the phonons involving energy and width. These results show $Co_2P_2S_6$, and its doped and 2D variants, will likely host as interesting physics as the Fe and Mn based counterparts.

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P2.116 UV-resistant Self-healing Emulsion Glass as a New Liquid-like Solid Material for 3D Printing

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Directly writing 3D structures into supporting mediums is a relatively new developing technology in additive manufacturing. In this work, durable and recyclable liquid-like solid (LLS) materials are developed as supporting mediums that are stable for both UV- and thermal-solidification. Our LLS material is comprised of densely packed oil droplets in a continuous aqueous medium, known as emulsion glass. Its elastic nature emerges from the jammed structure of oil droplets, which offers this LLS material rapidly self-healing ability. Moreover, the yield stress of the glass is relatively low and can be tuned by the viscosity and weight percentage of oil. The capability of the emulsion glass as supporting mediums is successfully demonstrated by directly writing and then curing designed structures. The emulsion glass has been repeatedly used at least 6 times upon exposure to UV irradiation and heat, implying it can expand the applications of supporting medium to the writing process involving UV- and thermal-curable inks simultaneously.[1]

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P2.118 A Journey Towards Azo-connected Covalent Organic Frameworks

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Covalent organic frameworks (COFs) are a class of crystalline organic solids possessing permanent porosity and high stability due to their strong covalent linkages.[1] Since the discovery of COFs in 2005, this area of research has expanded and resulted in over 297,000 publications to date. In contrast to the diverse structures, properties, and applications of COFs, the covalent bonds that link individual building units are scarce, with only 33 linkages documented in the literature.[2] The chemistry of these linkages is under-utilised when probing materials functions and applications. My research aims to create a new stable redox-active COF linkage via the post-synthetic modification of azodioxy- to azo- linkages. Theoretical specific capacity and modelling data suggests that these COFs will have large pores and possess redox active linkages. My results demonstrate the synthetic efforts we have made towards the synthesis of these azo-connected COFs.

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P2.119 A computational study on the activity and selectivity of single-atom catalysts for electrochemical reduction of N2 to NH3

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Ammonia (NH3) is one of the mostly heavily produced chemicals globally due to its primary use as a feedstock for nitrogenous fertilisers. For over a century, NH3 has been primarily produced by the Haber-Bosch process, which reacts gaseous nitrogen and hydrogen to form NH3, typically using a metallic catalyst. However, high pressures and temperatures are required, leading to this process consuming around 2 % of the global energy budget.1

Electrochemical methods of N2 reduction to NH3 (NRR) have been pursued in recent years, in which gaseous nitrogen reacts with solvated protons and electrons, rather than gaseous hydrogen, and an applied potential is used to drive the reaction. A catalyst is also required for this process, however for most traditional catalysts, the hydrogen evolution reaction (HER) outcompetes NRR, leading to very low Faradaic efficiency.2 Accordingly, much research is currently focussed on new classes of catalysts that do not suffer this lack of selectivity.

Single-atom catalysts (SACs) have been proposed as effective NRR catalysts. They have high reactivity due to their undersaturated coordination environment and maximum site specificity. Furthermore, they can, in principle, be tuned to favour NRR over HER. However, at present there exist very few design rules to enhance this selectivity. In the present study, systematic density function theory (DFT) studies of an Mo SAC on an MoS2 support are conducted to calculate NRR and HER activity. Analysis of the electronic structure of the SAC is performed to understand the observed trends in activity and selectivity.

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P2.120 High Solar Water Evaporation Rate using Silver Nanoparticles Decorated Diatom Frustules for Water Purification

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There is an ongoing crisis between the world's urban population growth and potable water shortage that has become one of the most challenging issues globally in the twenty-first century [1]. For this reason, there is considerable interest in developing new sustainable and environmental-friendly methods for water purification. One solution is using the solar water interfacial technique driven by solar energy [2]. The barrier to this technique is achieving a high evaporation rate. One way to enhance the evaporation rate is using a natural and renewable bio-material, diatom frustules, because of their porous nano- and micro-structured cell walls composed of hydrated silica [3]. One of the advantages of diatom frustules is their hydrophilic silica surfaces facilitating water transportation via capillary forces. However, the bio-silica of diatom frustules has weak light absorption, resulting in a low evaporation rate.

Herein, we report silver nanoparticle decoration of diatom frustules for solar water interfacial evaporation with a high evaporation rate. The nanoparticle synthesis was adapted from our method previously used to attach single layer silver nanoparticles to quartz substrates [4]. The monolayer of silver nanoparticle decorated diatom frustules exhibited a light absorbance of nearly 90% over the Vis-NIR range, covering most of the solar irradiance spectrum. The evaporation rate of a droplet with floating decorated diatom frustules under 1 sun was more than five times that of a bare water droplet. Our results show that Ag nanoparticle decorated diatom frustules have great potential for water purification to solve the future issue of water shortage.

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P2.121 Escherichia coli Detection Using Proteolytic Cleavage by Its Outer Membrane OmpT

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Various methods have been developed for the detection of Escherichia coli (E. coli); however, they are complex and time-consuming. OmpT (a cell membrane endopeptidase of E. coli) strongly embedded in the outer membrane of only E. coli, exposed to external solutions, with high proteolytic activity, could be a suitable target molecule for the rapid and straightforward detection of E. coli. Herein, a wash-free, sensitive, and selective amperometric method for E. coli detection, based on rapid and specific proteolytic cleavage by OmpT, has been reported. The method involved (i) rapid proteolytic cleavage of consecutive amino acids, after cleavage by OmpT, linked to an electrochemical species (4-aminophenol, AP), by leucine aminopeptidase (LAP, an exopeptidase), (ii) affinity binding of E. coli on an electrode, and (iii) electrochemical-enzymatic (EN) redox cycling. OmpT cleaved the intermediate peptide bond of a peptide substrate containing alanine-arginine-arginine-leucine-AP (−A-R-R-L-AP), forming R-L-AP, followed by the cleavage of two peptide bonds of R-L-AP sequentially by LAP, to liberate an electroactive AP. Affinity binding and EN redox cycling, in addition to rapid proteolytic cleavage by OmpT and LAP, enabled high electrochemical signal amplification. Two-sequential-cleavage was employed for the first time in protease-based detection. The calculated detection limit for E. coli cells in tap water (approximately 103 CFU/mL after 1 h incubation) was lower than those obtained without affinity binding and EN redox cycling. The detection method was highly selective to E. coli as OmpT is present in only E. coli. High sensitivity, selectivity, and the absence of wash steps make the developed detection method practically promising.

P2.122 High Performance Tri-Gate InAlN/GaN High-K MOSHEMTs with Light Fluorine Dopants

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In this work, we demonstrate a high performance tri-gate InAlN/GaN high-K MOSHEMTs with light fluorine dopants.

First, the device is a tri-gate nanowire structure with high work function metal and light fluorine dopants to achieve an enhancement-mode device.

In order to further improve the control ability of the gate, we use a tri-gate structure with high-k dielectric dual oxide layers. The high-k dielectric dual oxide layers have a high dielectric, which can enhance the control ability of the tri-gate and further improve the performance of the device. In addition, the strong electric field control ability can suppress the problem of thermal stability of fluorine ions at high temperature, so that the device remains highly reliable and stable at high temperature.

Moreover, we use the Schottky drain extension structure, whose function is like a drain field plate, which can effectively distribute the drain electric field and increase the breakdown voltage. In addition, the breakdown voltage is effectively improved while the on- resistance doesn't degrade due to Schottky drain extension with a low work function metal.

The device has a threshold voltage (VTH) of +0.48 V, an on/off current ratio of 1010, a sub-threshold swing (SS) of 67.3 mV/ten times, and an on-state current (Ion) of 810 mA/mm, at The breakdown voltage (VBR) at 1μA/mm is 630 V.Compared with traditional planars devices, all performances have been significantly improved.

P2.123 Predicting Ion Transport through Structurally Complex Graphene Oxide Structures

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Graphene oxide (GO) has the potential to be a low-cost material for water filtration and desalination. To maximize the potential of GO in this area, the structure/property relationships of GO need to be established, and molecular simulation is one way to accomplish this. However, in this field of molecular simulation, idealized GO structures are commonly used [1,2], which do not include holes and defects in the GO sheets. Here, a new computational method is introduced to create realistic GO sheets structure with extraordinary complexity that can be directly applied in molecular dynamics simulations [3]. Using this procedure, structurally-complex GO membrane stacks were computationally constructed. Different aspects of the GO membrane structure were investigated including the vertical distance between two adjacent layers (parallel to the GO membrane stacking direction, known as the interlayer spacing), the amount of water between each pair of layers, the presence of different holes in the sheets, and the lateral distance between two adjacent sheets located in the same stack layer. These aspects formed the basis of subsequent transport analyses of ions through the membrane, starting with permeation through a single perforated GO sheet. Free energy calculations of the permeation barrier indicate significant differences based on the chemistry of the hole edges, the hole size, and the ion type.

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P2.124 Fibrillar Surface Topography Modulates Corneal Keratocytes Fate and Behaviour

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Damaged cornea requires immediate treatment to prevent its disruption and possible vision loss. In the field of regenerative ophthalmology, the use of biochemically modified scaffolds is thought to be the most common way to address this issue whereas the influence of scaffold's mechanical properties requires further investigation.1-3 Here we tested the hypothesis that different fibrillar surface topographies would affect corneal keratocytes (KCs) fate and behaviour.

Type I collagen from rat tails mixed with HEPES buffer was used to create fibrillar collagen membranes (FCM). Human amniotic membranes (HAM) were used in comparison. The surface topography of both scaffolds was estimated by SEM. The impact of scaffold's surface topography on cultured KCs was evaluated via the analysis of focal adhesions (FAs) proteins rearrangements, changes in the extracellular matrix (ECM)-associated genes expression and protein synthesis, as well as KC's migration patterns. Tissue culture polystyrene (TCPS) was used as a control.

HAM comprised fibrils with a diameter of 248±7 nm. Meanwhile, FCM was composed of fibrils with a diameter of 71±3 nm. FCM's surface topography was found to promote the earlier FAs assembling followed by the earlier activation of mechanotransduction pathways leading to the increase of ECM proteins synthesis. Meanwhile, HAM's surface topography promoted the opposing effect resulting in the increase of KCs movement and reduction of ECM proteins deposition.

Overall, our findings elucidate the possible mechanism by which KCs could sense differences in fibrils diameter as well as connect these topographical features to the specific cell responses.

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2. Chen, Z.; You, J.; Liu, X.; Cooper, S.; Hodge, C.; Sutton, G.; Crook, J. M.; Wallace, G. G. Biomaterials for Corneal Bioengineering. Biomed. Mater. 2018, 13 (3), 032002. https://doi.org/10.1088/1748-605X/aa92d2.
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P2.125 Interfacial colloidal assembly guided by optical tweezers and tuned via surface charge.

Dr Susav Pradhan[1,2,5], Dr Catherine P Whitby[1,5], Dr Martin A K Williams[1,5], Dr Jack L Y Chen[3,4,5], Dr Ebubekir Avci[2,5]

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Poster Session 2 + Tech Tasters Pitch Sessions, February 8, 2023, 5:35 PM - 7:30 PM

The size, shape, and dynamics of assemblies of colloidal particles optically-trapped at an air–water interface can be tuned by controlling the optical potential, particle concentration, surface charge density and wettability of the particles and the surface tension of the solution.

The assembly dynamics of different colloidal particle types (silica, polystyrene and carboxyl coated polystyrene particles) at an air–water interface in an optical potential were systematically explored allowing the effect of surface charge on assembly dynamics to be investigated. Additionally, the pH of the solutions were varied in order to modulate surface charge in a controllable fashion. The effect of surface tension on these assemblies was also explored by reducing the surface tension of the supporting solution by mixing ethanol with water.

Silica, polystyrene and carboxyl coated polystyrene particles showed distinct assembly behaviours at the air–water interface that could be rationalised taking into account changes in surface charge (which in addition to being different between the particles could be modified systematically by changing the solution pH). Additionally, this is the first report showing that wettability of the colloidal particles and the surface tension of the solution are critical in determining the resulting assembly at the solution surface.

References:

1. Susav Pradhan et al. Interfacial colloidal assembly guided by optical tweezers and tuned via surface charge. Journal of Colloid and Interface Science, Volume 621, 2022, Pages 101-109, ISSN 0021-9797.
2. Lu et al. Optical Force-Induced Dynamics of Assembling, Rearrangement, and Three-Dimensional Pistol-like Ejection of Microparticles at the Solution Surface, J. Phys. Chem. C (2020)
3. R. Dasgupta et al. Trapping of micron-sized objects at a liquid-air interface. J. Opt. A: Pure Appl. Opt. (2007)

Oral Presentation Index

Presenting Author Names	Date	Paper Title	Type
Robert Abbel	Thur 9 Feb	5C.4 Conductive composites of an elastomeric biopolyester and their application in 3D printed sensor devices	Oral
Dr Susant Acharya	Thur 9 Feb	4C.2 Heusler Alloy-Based Magnetic tunnel Junctions with Perpendicular Easy Axis for Magnetoresistive Sensors	Oral
Dr Alireza Akbarinejad	Thur 9 Feb	5C.1 Biodegradable piezoelectric nanogenerators from biological materials	Oral
Dr Golrokh Akhgar	Wed 8 Feb	I3C.1 Introducing Disorder and Magnetism into Topological Materials	Invited
Professor Deji Akinwande	Tue 7 Feb	K.05 New Applications of 2D Materials from Wearable Health to Memory Devices and 6G Switches	Keynote
Dr. Kristi Anseth	Tue 7 Feb	Pl.02 Dynamic Hydrogel Matrices to Study Biology in the 4th Dimension	Plenary
Baptiste Auguie	Tue 7 Feb	I1B.2 Modelling light absorption in hybrid core-satellite metal nanostructures	Invited
Miss Patjaree Aukarasereenont	Tue 7 Feb	1C.3 Two-dimensional (2D) p-type semiconducting oxide from liquid metal alloy	Oral
Dr Ebubekir Avci	Tue 7 Feb	1E.1 Sustainable Solution for Gut Microbiota Sampling	Oral
Dr. Swarna Basu	Tue 7 Feb	I1A.2 Nanoscience Education as a Vehicle to Enhance Scientific Literacy	Invited
Dr Johnny Beaugrand	Thur 9 Feb	5A.2 A circular approach to valorize greenhouse tomato by-products in biobased and biodegradable injected materials for horticulture sectors	Oral
Professor David Beebe	Fri 10 Feb	I6A.2 Exclusive liquid repellency enabled under-oil open microfluidic systems	Invited
Miss Sara Beikzadeh	Wed 8 Feb	3A.4 Antibacterial and Antiviral Solid-State Carbon Cloth Supercapacitor	Oral
Mr. Shuva Bhowmik	Thur 9 Feb	5A.4 Bioactive biomaterials derived from chitosan for active and sustainable food packaging	Oral
Professor Ben Boyd	Wed 8 Feb	I2B.2 Metabolic labelling as a novel approach for targeting the gastrointestinal tract	Invited
Ms Diane Bradshaw	Tue 7 Feb	I1A.1 Te Tai Hauāuru O Te Ika Whenua – Convergence of West Coast terrestrial ecosystems from the great fish of Māui	Invited
DR. David Britt	Wed 8 Feb	2B.2 Targeted nano-formulations in agriculture: Lessons from medicine	Oral
Professor Sally Brooker	Wed 8 Feb	I3B.1 German-New Zealand: Green Hydrogen	Invited
Miss Lara Browne	Wed 8 Feb	3B.1 Exploring the potential for water-based upconversion to enhance hydrogen production by photolysis	Oral
Dr Saffron Bryant	Tue 7 Feb	1E.3 Deep Eutectic Solvents as Cryoprotective Agentsfor Mammalian Cells	Oral
Professor Gary Bryant	Fri 10 Feb	6E.1 Measurement of Cell Motility using Differential Dynamic Microscopy (DDM)	Oral
Dr Philip Brydon	Fri 10 Feb	I6C.3 A natural surprise: The superconductivity of Rh17S15	Invited
Dr. Chris Bumby	Thur 9 Feb	I5B.1 Zero-CO2 ironmaking in a hydrogen fluidised bed	Invited

Professor Weibo Cai	Fri 10 Feb	I6A.3 (Cancer) Theranostics with Radiolabeled Nanomaterials	Invited
Miss Yueying Cao	Wed 8 Feb	2E.5 Real-Time Imaging of Nanoparticle Transcytosis in a Microfluidic Blood–Brain Barrier Model	Oral
Dr Anaïs Chalard	Tue 7 Feb	1E.2 Stiffness-patterned and hierarchical GelMA hydrogels towards in vitro cardiac scar tissue models	Oral
Dr Kai Chen	Wed 8 Feb	2C.5 Ultrafast photoexcitation dynamics in ternary organic solar cells	Oral
Dr Yi Chen	Fri 10 Feb	6E.4 Sustainable electronics with carbon nanofibres for flexible sensor applications	Oral
Professor Rebecca Cheung	Tue 7 Feb	K.02 Integration of low dimensional materials for sensing applications	Keynote
Prof Jared Cole	Fri 10 Feb	6C.2 Using nano-electronics as a tool in materials science: unravelling the mystery of two-level defects in amorphous solids	Oral
Dr Michelle Cook	Tue 7 Feb	1B.3 Something about bubbles - a novel system design for testing catalysts for PEM/AEM electrolysis in an approximated MEA stack	Oral
Alexander Cook	Wed 8 Feb	3E.2 Exosome inspired RNA compartmentalisation in complex systems	Oral
A/prof. Dimitrie Culcer	Fri 10 Feb	I6C.2 Electrically-induced spin torques due to the bulk states of topological insulators	Invited
Glebert Dadol Pamela Mae Ucab	Fri 10 Feb	6A.4 Desalination Performance of a Passive Solar-Driven Membrane Distiller: Effect of Middle Layer Material and Thickness	Oral
Dr Torben Daeneke	Tue 7 Feb	1C.1 Liquid metal-based synthesis of functional 2D materials for electronic applications	Oral
Dr Nathaniel Davis	Tue 7 Feb	1D.1 Hybrid organic/inorganic nanomaterials - A new type of optoelectronic material.	Oral
Ms Xiaoxuan Deng	Wed 8 Feb	2B.4 Fabrication and characterisation of drug-eluting bioabsorbable surgical sutures	Oral
Mrs. Mantra Dheendayal	Thur 9 Feb	4B.1 Enhancing regeneration kinetics by tailoring the structure of the donor systems in organic dyes	Oral
Dr Shalini Divya	Wed 8 Feb	2A.2 TasmanIon: Moving towards sustainable aluminium-ion batteries	Oral
Professor Alexandre Dmitriev	Wed 8 Feb	I2D.2 Nanoscale magnetophotonics	Invited
Dr Huan Doan	Fri 10 Feb	6B.1 Novel hierarchical copper-based metal-organic frameworks for improved catalytic performance	Oral
Dr Timothy Duignan	Wed 8 Feb	2C.4 Towards predictive design of electrolyte solutions by accelerating ab initio simulation with neural networks.	Oral
Mr Samuel Edens	Thur 9 Feb	4B.3 Pure and mixed gas adsorption kinetics of ethylene and ethane in Mordenite, Zeolite 13X and ZJU-74a.	Oral
Dr. Aaron Elbourne	Thur 9 Feb	4E.1 Dynamics and Behaviour of Ultra-Small Gold Nanoparticles at Bio-Membranes – Combining Experiment with Simulation	Oral
Professor Amanda Ellis	Thur 9 Feb	K.16 3D printed fluoropolymers: From Energy Harvesting to Microfiltration	Keynote
Dr Courtney Ennis	Tue 7 Feb	1B.2 Vibrational analysis of host-guest interactions in porous materials as revealed by synchrotron infrared and DFT studies.	Oral

Mrs. Sana Fathima T K	Tue 7 Feb	1B.4 Development Of Non-Noble Metal Based Catalysts For Hydrogen Production By Seawater Electrolysis	Oral
Prof. Dr. Holger Fehske	Fri 10 Feb	6C.1 Quantum transport in a background medium: Fluctuations versus correlations	Oral
Dr Holger Fiedler	Wed 8 Feb	3B.3 Ion beam synthesis of metastable, high temperature transition metal carbides at room temperature	Oral
Ms Roslyn Forecast	Wed 8 Feb	3D.3 Triplet-Triplet Annihilation: Magnetic Field Effects in Solution	Oral
Prof Michael Fuhrer	Wed 8 Feb	I3C.2 The Topological Transistor as a Low-Voltage Switch	Invited
Dr. Aiko Fukazawa	Wed 8 Feb	K.08 Design of Novel Nonbenzenoid π-Electron Systems toward Unusual Yet Stable Functional Materials	Keynote
Professor Shuhei Furukawa	Fri 10 Feb	I6B.3 Metal-organic cage assemblies for gel engineering	Invited
Associate Professor David Garrett	Tue 7 Feb	I1E.2 Development progress towards a diamond and carbon fibre brain implant for epilepsy management	Invited
Professor Nicola Gaston	Tue 7 Feb	1C.2 Atomistic control for self-assembly of nanostructure	Oral
Professor Pieter Geiregat	Wed 8 Feb	3D.2 Optical Gain Spectroscopy of Nanostructured Materials: Bigger is Better	Oral
Dr Amy Gelmi	Thur 9 Feb	15E.1 External Stimulation Platforms for Stem Cell Fate Control	Invited
Judith Glasson	Wed 8 Feb	2E.2 Crystallins to Keratoplasties: Improving Biomimetic Corneal Stromal Materials	Oral
Dr Lucy Gloag	Thur 9 Feb	I4B.1 Synthesis of hierarchical metal nanostructures with high electrocatalytic surface areas	Invited
Mr Calum Gordon	Thur 9 Feb	5D.1 Performance Evaluation of Solid State Luminescent Solar Concentrators based on InP/ZnS–Rhodamine 101 Hybrid Inorganic-Organic Luminophores	Oral
Professor Keith Gordon	Fri 10 Feb	6B.3 Using metal complexes to open the door to long-lived excited states	Oral
Dr Renee Goreham	Thur 9 Feb	I5C.1 Quantum dots and extracellular vesicles as detection strategies for disease and bacteria	Invited
Prof Michele Governale	Fri 10 Feb	6C.4 Topological-Insulator Nanocylinders	Oral
Dr Florian Graichen	Thur 9 Feb	I5A.1 Linear to Circular Bioeconomy – New Zealand's opportunities and challenges in the 21st century	Invited
Dr Simon Granville	Thur 9 Feb	I4C.1 Topology and magnetism in Heusler alloy Co2MnGa – outstanding magnetoelectronic properties for physics and applications	Invited
Mr Jake Hardy	Thur 9 Feb	5D.4 Ruddlesden-Popper Mixed-Dimensional Perovskites for Triplet-Triplet Annihilation and Singlet Fission	Oral
Pauline Harris	Tue 7 Feb	Pl.01 Growing a Mātauranga Māori space in the MacDiarmid Institute	Plenary
Dr Azadeh Hashemi	Thur 9 Feb	15E.2 Directing the differentiation of stem cells using cell-imprinted culture platforms	Invited
Mr Zeger Hens	Tue 7 Feb	I1D.2 III-V Quantum Dots, Seeing Light and Dark	Invited
Mr Zachary Heywood	Thur 9 Feb	4D.2 Brain-like properties of percolating networks of nanoparticles	Oral
Professor Justin Hodgkiss	Thur 9 Feb	K.15 The photoprotection mechanism in the black-brown pigment eumelanin	Keynote
Dr William Holmes-Hewett	Wed 8 Feb	3A.1 Rare earth nitrides: From the lab to the world	Oral
Mr Matthew Horrocks	Thur 9 Feb	5E.2 Biomolecule incorporation and release from engineered biointerfaces for cell behavioral studies.	Oral

Miss Ringahora Huata	Tue 7 Feb	1A.1 Ngā Wai Ariki O Whakarewarewa He Kohikohinga Hau Kāinga - Perspectives, partnerships social-natural hazard materials of geothermal taonga	Oral
Prof Patricia Hunt	Wed 8 Feb	I2C.1 Ionic liquid systems: exploring partial charges, charge transfer and polarizability.	Invited
Prof. Luiz Jacobsohn	Wed 8 Feb	I3D.1 Thermoluminescence of MgAl2O4 and ZnAl2O4 Spinels	Invited
Chennupati Jagadish	Thur 9 Feb	Pl.04 Semiconductor Nanostructures for Optoelectronics Applications	Plenary
Mr Kumar Debajyoti Jena	Wed 8 Feb	3B.4 Synthesis of nano-structured Li4Ti5O12 via a superhydride-driven wet chemistry method as a highly sustainable anode material for lithium-ion batteries	Oral
Dr. Paul Jerabek	Wed 8 Feb	I3B.2 Metal Hydride Materials for Solid-State Hydrogen Storage Applications: Utilizing the Synergy of Experiment & Theory for Materials Design Challenges	Invited
Róisín Mooney Dr Marcus Jones	Fri 10 Feb	6D.3 Plasmon-enhanced optical properties of molecular chromophores coupled with size-tuned silver nanoparticles	Oral
Professor Jinsoo Joo	Fri 10 Feb	6D.1 Photo-triggered Charge Transfer of 2D-TMD-based Heterostructures: Implications in Exciton Optoelectronics	Oral
Mr Ajay Jose	Thur 9 Feb	5C.2 Synthesis and characterization of antimicrobial colloidal polyanilines	Oral
Dr Vedran Jovic	Thur 9 Feb	I4B.3 What makes Ruthenium Dioxide a benchmark electrocatalyst for the water splitting reaction? Root causes from a condensed-matter physics perspective	Invited
Prof. Hyun Young Jung	Wed 8 Feb	2C.2 Polysulfide Sieving Strategy through Tunable Ultralight Catalytic Interlayer for Stable Li-S Battery	Oral
Professor Kourosh Kalantar-Zadeh	Wed 8 Feb	K.09 Low melting point liquid metals based on post transition metals	Keynote
Dr. Richard Kaner	Wed 8 Feb	K.10 Hydrophilic Zwitterionic Polymer Coatings for Preventing the Adhesion of Bacteria on Medical Grade Polymers	Keynote
Professor Hong Seok Kang	Tue 7 Feb	1B.1 Phase Transition and Electrocatalytic Performance of Dichalcogenides of Transitions Metal Alloys	Oral
Dr Bushra Anam Khalil	Thur 9 Feb	4A.2 A comprehensive first-principles investigation on the defect chemistry of high performance lead-free BZT-BCT ferroelectric material	Oral
Sami Khan	Wed 8 Feb	3A.2 Boosting the Performance and Longevity of CO2 Capture and Conversion using Micro-nano Engineered Gas-Capturing Surfaces	Oral
Ph. D. Dongwook Kim	Thur 9 Feb	5D.2 Theoretical studies of thermally activated delayed fluorescence (TADF) emitters: Exciplex-type and multiple resonance type emitters.	Oral
Professor Jin Young Kim	Thur 9 Feb	5D.3 High-performance colorful semitransparent organic solar cells	Oral
Harm-Anton Klok	Wed 8 Feb	I2E.2 Chemical design of functional materials via surface-initiated polymerization	Invited
Professor Marc Knecht	Thur 9 Feb	4A.3 Bio-Inspired Approaches Towards Graphene/h-BN Nanosheet Assembly Under Sustainable Conditions	Oral
Dr Andrea Kolb	Tue 7 Feb	1A.2 Knowing and growing a student's strengths profile: How to assess and enhance transferrable skills in a university student	Oral
Professor Michael Kozicki	Thur 9 Feb	I4D.2 Dendrites as Digital Triggers	Invited

Professor Zdenka Kuncic	Thur 9 Feb	I4D.1 Neuromorphic properties of nanowire networks	Invited
Dr. Stephan Kupfer	Wed 8 Feb	I3B.3 The Rocky Road Towards Earth-Abundant Metals in Photocatalysis – A Quantum Chemical Perspective	Invited
Dr Girish Lakhwani	Fri 10 Feb	I6D.1 Perylene derivatives for polariton lasing	Invited
Dr Stephanie Lambie	Thur 9 Feb	5B.4 Characterising the structure and dynamics of liquid GaAu	Oral
Dr Deler Langenberg	Wed 8 Feb	2D.2 New Developments in Electronic Structure Investigation: Combining APRES and Microscopy Solutions	Oral
Dr Frédéric Laquai	Thur 9 Feb	15D.1 Interfacial Energetic Landscape in Non-fullerene Acceptor Organic Solar Cells and its Impact on Device Performance	Invited
Dr Marie-Joo Le Guen	Thur 9 Feb	I4E.3 3D printing cellulose: the influence of process parameters on crystal alignment	Invited
Dr Maxime Le Ster	Fri 10 Feb	6A.2 Moiré superlattices in reciprocal space	Oral
Lawrence Lee	Wed 8 Feb	I3E.3 Design and synthesis of 'smart', self-assembling molecular subunits with DNA origami	Invited
Dr. Dominik Legut	Thur 9 Feb	4C.3 Magnetism, magneto-elasticity, and magnetostriction at 3D/2D and at interfaces	Oral
Jérôme Leveneur	Wed 8 Feb	I2A.2 Bringing ion beams out of the lab	Invited
Dr. Peng Li	Wed 8 Feb	2B.3 Eco-friendly nanocarriers actualise biomolecule agrochemicals in crop production	Oral
Dr Jiaxin Lian	Fri 10 Feb	6E.2 A transparent platform for cell capture and single cell isolation	Oral
Sierin Lim	Fri 10 Feb	16E.1 Protein Assemblies at Interfaces: Fundamentals and Opportunities	Invited
Dr. Mutjalin Limlamthong	Thur 9 Feb	4B.2 Tuning alkane/alkene adsorption separation selectivity through acidic H-ZSM-5 zeolites	Oral
Dr Lujia (Luke) Liu	Wed 8 Feb	3A.3 A High-Valent Organic Linker-Based Metal-Organic Framework for Selective Methane Capture	Oral
Prof. Dmitri Louzguine	Wed 8 Feb	2D.1 Atomic structure of metallic glasses studied by synchrotron-radiation X-ray diffraction, scanning tunneling microscopy and ab-initio molecular dynamics simulation	Oral
Dr Yiqing Lu	Fri 10 Feb	6E.3 Real-time monitoring of cancer cell metastasis in mice using lanthanide nanoparticles	Oral
Dr Nigel Lucas	Fri 10 Feb	6B.2 Robust organic cages from cavitands: construction and cargo logistics	Oral
Professor Digby Macdonald	Thur 9 Feb	I5A.2 The Scientific Basis of Our Reactive Metals Based Civilization	Invited
Prof Stefan Maier	Fri 10 Feb	16D.3 Plasmonic and dielectric nanostructures for enhanced light harvesting, emission control, and nanometrology	Invited
Dr Sharali Malik	Fri 10 Feb	6A.1 Tubular glassy carbon microneedles with fullerene-like tips for biomedical applications	Oral
Dr Ben Mallett	Wed 8 Feb	3C.1 Thin-film multilayers of the high-temperature superconductor YBa2Cu3O7 and manganates RMnO3	Oral
Professor George Malliaras	Tue 7 Feb	K.03 Technology for Bioelectronic Medicine	Keynote
Miss Abigail Mann	Thur 9 Feb	5C.3 The exploitation of dynamic S-S bonds in 50-poly(S-r-DCPD) for erasable data storage and encoding messages	Oral
Prof. Smaranda Marinescu	Thur 9 Feb	K.13 Conductive Dithiolene-Based Metal-Organic Frameworks for Electrocatalytic H2 Production	Keynote
Dr. Colleen Marlow	Tue 7 Feb	1A.3 Research mentoring to increase diversity in STEM	Oral

Professor Aaron Marshall	Tue 7 Feb	1A.4 Hydrogen: An opportunity to teach thermodynamics	Oral
Dr Jacob Martin	Wed 8 Feb	2D.4 Peering into the Computational Microscope: Insights from 3D printing through to virtual reality	Oral
Dr Jitendra Mata	Wed 8 Feb	3E.3 Structural Characterisation of Silk Fibroin Based Hydrogels Using Small and Ultra-Small Angle Neutron Scattering Techniques.	Oral
Prof Sally McArthur	Tue 7 Feb	K.06 Characterisation of 3D cell cultures systems - challenges and opportunities	Keynote
Dr Davide Mercadante	Fri 10 Feb	I6E.3 Coevolution-driven and likelihood-based design of proteins for industrial applications.	Invited
Prof. Adam Micolich	Fri 10 Feb	I6B.1 A device-based approach to measuring the electrical conductivity of microscale metal-organic-framework (MOF) single crystals	Invited
Mr. Kirill Misiiuk	Thur 9 Feb	4E.3 Topographical surface tension gradients for passive motion of water micro-droplets	Oral
Dr Sheikh Mohamed Mohamed	Wed 8 Feb	2E.4 In Vitro Trans-Blood Brain Barrier Delivery of Neurotrophin Loaded Nanoparticles to Address Neuronal Damage	Oral
Mrs Nur Maizura Mohd Darbi	Wed 8 Feb	3E.1 Toxicity and selectivity studies of linear lipopeptide battacin analogues using model membrane	Oral
Dr Vanessa Morris	Fri 10 Feb	I6E.2 Amyloid fibril proteins: health, disease and applications	Invited
Ms Stephanie Mudd	Wed 8 Feb	3C.4 Reducing Thermal Conductivity in n-type Thermoelectric Oxides Using a Novel Cold Sintering Process	Oral
Professor Bhaskaran Muralidharan	Fri 10 Feb	6C.3 "topotronics" with 2D-Xenes - from quantum matter to emerging devices	Oral
Prof. Tomonobu Nakayama	Wed 8 Feb	I3C.3 Materials Nanoarchitectonics: The World-Smallest Car Race to Artificial Brain	Invited
Dr Franck Natali	Wed 8 Feb	I3A.2 Facile dissociation of molecular nitrogen using lanthanide surfaces: Towards ambient temperature ammonia synthesis	Invited
Miss Linh Nguyen	Thur 9 Feb	5E.1 Gelatin methacryloyl microspheres to enhance the survival and maturation of directly reprogrammed neurons for cell replacement therapy in Huntington's Disease	Oral
Dr Michel Nieuwoudt	Fri 10 Feb	I6A.1 Shedding light on skin cancers and skin diseases with Raman spectroscopy	Invited
AA/Prof. Dr.-Ing. Jens Noack	Wed 8 Feb	I2C.2 Tools for the search of new organic active materials for new redox flow batteries	Invited
Dr Dipl-Ing Volker Nock	Wed 8 Feb	I2B.1 Microfluidics at the interface of plants and pathogens	Invited
Dr Emilia Nowak	Thur 9 Feb	I4E.1 Dynamics at the interfaces & spontaneous motions in liquid-liquid and gas-liquid-solid systems	Invited
Professor David Officer	Thur 9 Feb	4A.1 Highly Processable Edge Functionalised Graphene: From Dough to Dispersions	Oral
Daniel Packwood	Thur 9 Feb	I4A.3 In-silico prediction of functional on-surface supramolecular materials	Invited
Elke Pahl	Thur 9 Feb	I4A.1 Melting in Extreme Environments Using Monte Carlo Simulations	Invited
Nathan James Pataki	Wed 8 Feb	2A.4 A scalable solution-processed organic thermoelectric generator with record high thermocouple density	Oral
Mr Shae Patel	Fri 10 Feb	6B.4 MOFs for CO2 Electroreduction	Oral
Dr Natalie Plank	Wed 8 Feb	K.07 Carbon Nanotube Field Effect Transistor Platforms for Sensitive and Real-time Sensing	Keynote

Ms Catherine Pot	Thur 9 Feb	4C.1 Switchable Magnetic Dots for Cryogenic MRAM	Oral
Prof Annie Powell	Wed 8 Feb	I2D.1 Setting spins into a spin – single molecule toroidal systems	Invited
Dr. Vinich Promarak	Wed 8 Feb	3D.1 Deep Blue-Emissive Molecules With Combined Hot Exciton and Aggregation-induced emission (AIE) Features as Efficient Emitters for Non-Doped OLEDs	Oral
Dr Susan Quinn	Fri 10 Feb	K.18 Resolving the Light-Activated Processes of DNA Bound Transition Metal Polypyridyl Complexes Towards Imaging and Therapeutic Applications	Keynote
Dr. Marilou Raduban	Wed 8 Feb	I3D.2 Wide band gap nanoparticle thin films as photoconductive sensors of high-energy radiation	Invited
Professor Michael Reid	Wed 8 Feb	3C.2 Zeeman Interactions in Rare-Earth Doped Nanocrystals	Oral
Dr Haoran Ren	Fri 10 Feb	6D.2 Metafibre Optics: Principles, Fabrication, and Applications	Oral
Charles Royal	Tue 7 Feb	K.01 Science and Mātauranga Māori: Some Thoughts	Keynote
Dr Daniel Sando	Thur 9 Feb	I4D.3 Anisotropic epitaxial stabilization of a low-symmetry ferroelectric with enhanced electromechanical response	Invited
Professor Maciej Sawicki	Thur 9 Feb	I4C.2 Towards spintronics functionalization of nitrides	Invited
Professor Mathieu Sellier Mr Finn McIntyre	Wed 8 Feb	2D.5 Spin coating curved surfaces: simulation and experiments	Oral
Dr. Kai Sellschopp	Wed 8 Feb	3B.2 Computational Recipes for High-Throughput Screening of Metal Hydrides for Hydrogen Storage	Oral
Mx Zo Shaw	Thur 9 Feb	5E.3 Eutectic gels with 2D black phosphorus nanoflakes for antimicrobial treatments	Oral
Dr Jami Shepherd	Wed 8 Feb	I3A.3 Quantifying flow in bone with ultrasound and photoacoustic imaging	Invited
Dr Peter Sherrell	Thur 9 Feb	5A.1 Harvesting (and Using) Motion via Polymers	Oral
Dr Georgina Shillito	Tue 7 Feb	I1B.1 Uncovering electron transfer pathways: towards the rational design of light-harvesting molecules	Invited
Professor Michelle Simmons	Fri 10 Feb	Pl.06 The physics of quantum processors: making machines at the atomic-limit	Plenary
Dr. Sean Simpson	Wed 8 Feb	I2A.1 Enabling a Circular Economy: Carbon-Negative Fuel and Chemical Production by eliminating waste	Invited
M. Cather Simpson	Wed 8 Feb	2B.5 Raman spectroscopy and chemometric analysis in phytoplankton monitoring	Oral
M. Cather Simpson	Wed 8 Feb	Pl.03 Academic Entrepreneurship – Selling Out or Delivering Value?	Plenary
Mr Fernando Solis Fernandez	Wed 8 Feb	3D.4 Optical Fiber Sensors in Tokamak Fusion Reactors	Oral
Arya A. Soman	Wed 8 Feb	3C.3 Designing high-performance superconducting thin films using ion beam technology	Oral
Prof. Seung-Wan Song	Wed 8 Feb	2C.1 Interface Stabilization as a Key for Promoted Safety and Energy Density of Nickel-rich Cathode Material-based Lithium-ion Batteries	Oral
Professor Nicola Spaldin	Thur 9 Feb	I4C.3 Multiferroics beyond electric-field control of magnetism	Invited
Professor Kathleen Stebe	Thur 9 Feb	Pl.05 Active colloidal particles in nematics for physically intelligent micro-robotics and reconfigurable materials	Plenary
Dr. Krista Grace Steenbergen	Tue 7 Feb	I1C. 1 Remarkable nano-patterning in liquid metals	Invited
Dr Hannah Stern	Wed 8 Feb	I3D.3 Identification of single optically addressable spins in a two-dimensional material.	Invited

Dr. Michael Susner	Thur 9 Feb	I4A.2 Functional van der Waals Materials: A New Avenue for Next-Generation Electronics	Invited
Professor Duncan Sutherland	Thur 9 Feb	K.14 Dynamic protein coatings modulate nanomaterials interactions in the context of nanotoxicology and nanomedicine	Keynote
A/Prof Darren Svirskis	Tue 7 Feb	I1E.1 A Subdural Bioelectronic Implant for use following Spinal Cord Injury in Rats	Invited
Brandon Swanepoel	Wed 8 Feb	I3A.1 Waste as a resource… a rethink	Invited
Dr Nitu Syed Dr Azmira Jannat	Tue 7 Feb	1C.4 Liquid metal derived atomically thin indium nitride (InN) films featuring 2D electron gases	Oral
Dr Jianbo Tang	Tue 7 Feb	I1C.2 Surface-Grown Crystalline Patterns and Structures from Liquid Metal Solvents	Invited
Prof Junwang Tang	Thur 9 Feb	I4B.2 Conversion of CH4 to high value chemicals by photocatalysis	Invited
Dr Ayelen Tayagui	Wed 8 Feb	2B.1 Studying the growth of oomycetes in an oxygen gradient on chip	Oral
Professor Richard Taylor	Fri 10 Feb	K.19 Controlled assembly of retinal cells on fractal and Euclidean electrodes	Keynote
Shane Telfer	Wed 8 Feb	2A.1 The KakaPore start-up: Capturing carbon dioxide	Oral
Dr. Raweewan Thiramanas	Wed 8 Feb	2E.3 Bio-functionalization of titanium dioxide nanoparticles surface for controlling their cellular uptake in skin cells	Oral
Dr Mi Tian	Thur 9 Feb	5A.3 Ball-Milling for the Green Synthesis of Metal-Organic Frameworks: a Design-of-Experiment Approach	Oral
Benjamin Tilmann	Tue 7 Feb	1D.3 Gallium Phosphide nanostructures as versatile platform for nonlinear and ultrafast nanophotonics	Oral
Professor Yuye Tong	Fri 10 Feb	I6B.2 Operando Infrared and Nuclear Magnetic Resonance Methodologies for Probing Chemistry of Working Batteries	Invited
Professor Matt Trau	Wed 8 Feb	I2E.1 Some new nanotechnologies for applications in cancer and immunotherapy	Invited
Dr Lorenzo Travaglini	Wed 8 Feb	3E.4 Controlled Spatial Fabrication of Metalloprotein Nanostructures for Bio-Interfacing	Oral
Prof Jadranka Travas-Sejdic	Thur 9 Feb	I5C.2 Novel conducting polymers biointerfaces for bioelectronics	Invited
Eddyn Treacher	Thur 9 Feb	4D.1 Behaviour of Ag-Ag2S-Ag Atomic Switch Networks with the Addition of a Carbon Nanotube Network Layer	Oral
Professor Antonio Tricoli	Fri 10 Feb	I6D.2 Engineering Scalable Electrocatalysts for Affordable Production of Green Hydrogen	Invited
Dr. Ilia Valov	Wed 8 Feb	K.12 New mechanism in memristors revealed – prospective and challenges	Keynote
Ajayan Vinu	Fri 10 Feb	K.17 Nanoporous materials with different functional elements: unique materials with multiple functions	Keynote
Dr Isabella Wagner	Thur 9 Feb	15D.2 Accumulation of Dark Excitons in Thin Quasi-2D Perovskites Limits Amplified Spontaneous Emission	Invited
Prof Sumeet Walia	Tue 7 Feb	I1D.1 Two-dimensional materials for next-generation electronics and optoelectronics technologies	Invited
Prof Tiffany Walsh	Wed 8 Feb	K.11 Guiding Peptide-driven Exfoliation and Organization of 2D Nanomaterials	Keynote
Professor Xiaolin Wang	Tue 7 Feb	K.04 The grand design of new class of materials and properties	Keynote
Prof Gregory Warr	Thur 9 Feb	I4E.2 Amphiphilic Self-Assembly Structure and Dynamics in Ionic Liquids	Invited

Dr Geoffrey Weal	Thur 9 Feb	5B.3 Data-Driven Structure-Function Mapping of Organic Solar Cell Materials	Oral
Yu-Chen Wei	Tue 7 Feb	1D.4 Single-mode THz vibronic coherence contributes to suppression of nonradiative rates in molecular aggregates	Oral
Geoff Willmott	Thur 9 Feb	4E.2 Unusual Geometries Following Drop Impacts Using Advanced Materials	Oral
Professor Han Young Woo	Fri 10 Feb	6A.3 Homojunction organic thin film transistors by selective molecular doping	Oral
Prof Tim Woodfield	Wed 8 Feb	I3E.2 See the Light: Advanced Light Activated Materials for 3D Bioprinting & Regenerative Medicine	Invited
Research Director Natasha Wright	Wed 8 Feb	2D.3 Holistic approaches to Advanced Characterisation of Novel Materials	Oral
Mr Steven Wu	Wed 8 Feb	2A.3 Effect of processing conditions on suspension polymerization reaction of molecularly imprinted adsorption media	Oral
Dr Ting Wu	Thur 9 Feb	5B.2 Electrochemical CO2 extraction from seawater	Oral
Dr Amy Yewdall	Wed 8 Feb	I3E.1 Phase tools for synthetic biology: shaping condensate dynamics with ATP:Mg2+	Invited
Prof. Jeongsoo Yoo	Wed 8 Feb	2E.1 PEGylated liposome encapsulating nido-carborane: boron neutron capture therapy (BNCT) and in vivo trafficking study by PET imaging in animal models	Oral
Soongil Yoon	Thur 9 Feb	4D.3 Transfer-free n- and p-channel graphene field-effect transistors using graphene grown directly at 100 oC	Oral
Ali Zavabeti Ms. Linlin Ye	Thur 9 Feb	5B.1 Carbon Dioxide Conversion Using Low Melting point Gallium Magnesium Liquid Metal Alloys	Oral
Chase Zemke-Smith	Tue 7 Feb	1D.2 Whispering Gallery Mode Lasing from Perovskite Nanocrystals Chemically Attached to Microcavities	Oral
Clara Zens	Wed 8 Feb	2C.3 Tailoring charge transfer processes in organic radical batteries	Oral
Dr Jie Zhang	Thur 9 Feb	I5B.2 Electrochemical Reduction of Carbon Dioxide	Invited
Kaiwen Zhang	Tue 7 Feb	1E.4 Temporal analysis of human mesenchymal stem cells under electrical stimulation with AFM	Oral
Peikai Zhang	Wed 8 Feb	2A.5 Wet-printing of Conformable and Stretchable Conducting Polymer Microelectrode Arrays for Gastric Slow Wave Recording	Oral
Yi (Ethan) Zhang	Thur 9 Feb	5E.4 Characterisation of collagen: the use of synchrotron small-angle X-ray scattering (SAXS) and surface-enhanced Raman spectroscopy (SERS)	Oral
Prof Ulrich Zuelicke	Fri 10 Feb	I6C.1 What happens when you make a quantum well antiferromagnetic?	Invited

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Dr Geoffrey Weal	Tue 7 Feb	Data-Driven Structure-Function Mapping of Organic Solar Cell Materials	P1.112
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Dr Ben Westberry	Tue 7 Feb	Structural Studies of Amorphous Systems Using Molecular Dynamics Simulations and X-ray Scattering Experiments: Developing Models for the Carrageenan Disorder-Order Transition	P1.109
Mr. John Whiting	Wed 8 Feb	A computational study on the activity and selectivity of single-atom catalysts for electrochemical reduction of N2 to NH3	P2.119
Isabelle Williams	Tue 7 Feb	Development and implementation of a multi-spectroscopic platform for the identification and biochemical characterization of cellular differences found in phytoplankton communities	P1.115
Joey Williamson	Tue 7 Feb	Magnetic study of CoMoO4: observation of a spin flop transition	P1.116
Miss Kate Wislang	Tue 7 Feb	Properties of Sn- and Si-Doped Gallium Oxide Thin Films Produced Using Sol-Gel Techniques	P1.117
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