

Newcastle

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Newcastle – Keynote Abstracts

From froth flotation on Earth to electrostatic beneficiation on the Moon: The route towards dry mineral processing

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On Earth, froth flotation is a hugely successful process to separate minerals, consuming large quantities of water and producing vast amounts of tailings. On the Moon, the production of small quantities of oxygen or water in the next 5 years will mark a new era for human space travel. Although seemingly unlinked, the success of both flotation and lunar oxygen production is related to mineral surface properties. Furthermore, bringing together the space resources and mineral processing sectors brings a fresh perspective to our terrestrial operations, particularly with respect to water use. In this talk, we will look at methods of separating Moon dust based on electrostatic properties, and consider how this might enable the transformation of mineral processing from wet to dry.

Biography

Dr Kathryn Hadler is a lecturer in the Department of Earth Science and Engineering at Imperial College London. Her primary field of research has been optimising froth flotation performance, particularly through numerous industrial experimental trials. In recent years, she has focused on the removal of water from mineral processing operations and the transition to dry processing on Earth, and the use of beneficiation techniques on the Moon. She leads the European Space Agency Topical Team on space resource utilisation.

Rational Design of Poly(ethylene glycol) Nanoparticles for Targeted Drug Delivery

Jiwei Cui

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Biography

Jiwei Cui is a professor in the Key Laboratory of Colloid and Interface Chemistry of the Ministry of Education at Shandong University in China. He received his Ph.D. in colloid and interface chemistry from Shandong University in 2010 and worked as a research fellow at The University of Melbourne during 2010-2016. He was awarded as an ARC Super Science Fellow in 2011 and was selected as a Young Talent Fellow in China in 2016. His research interests include colloidal assembly, interface engineering, polymer hydrogels, drug and vaccine delivery.

Robert Chapman

Abstract

Successful accumulation of drugs specifically at diseased sites is mainly limited by biological barriers, especially the nonspecific uptake of drug carriers in mononuclear phagocyte system (MPS). Hence, it is critical to develop drug delivery systems that can specifically bind to diseased cells, while avoiding interactions with normal, healthy cells. This presentation will demonstrate the rational design of polymer particles mainly composed of poly(ethylene glycol) (PEG), and will show the cell association and biodistribution of these particles, as well as cell targeting of PEG particles modified with targeting molecules for drug delivery. The optimization of PEG particle engineering to overcome the MPS biological barrier for efficient tumour targeting in mouse studies is examined by tuning PEG molecular weight, particle size, particle stiffness, and targeting moieties, which highlights the influence of unique aspects of polymer particles on biological interactions. The reported PEG particles represent a new type of polymer carriers with potential biomedical applications.

Colloids for signal amplification in biosensing

Dr Robert Chapman

Biography

Dr Chapman is a Lecturer in Chemistry in the School of Environmental and Life Sciences, and an adjunct lecturer in the School of Chemistry at UNSW. His research focusses on the use of high throughput polymerisation techniques to design polymer therapeutics. He has expertise in a broad range of polymer chemistry, peptide driven self-assembly, drug delivery, tissue engineering and in nanoparticle based biosensing. Prior to joining the University of Newcastle, Dr Chapman completed a BEng in Industrial Chemistry (2002-07) at UNSW. After a year working in management consulting for the Boston Consulting Group, he moved to the University of Sydney for his PhD in Chemistry (2009-12) under Profs. Sebatien Perrier and Katrina Jolliffe, where he studied the synthesis and self-assembly of cyclic peptide - polymer conjugates. From 2013-15 he worked as a research associate in the lab of Prof. Molly Stevens at Imperial College London on the development of nanomaterial based biosensors and scaffolds for tissue engineering. He then returned to the School of Chemistry at UNSW to begin his independent career as a Vice-Chancellors Research Fellow (2016) and DECRA fellow (2017-20), before moving to the University of Newcastle in 2020.

Abstract

The ability to engineer and control structure on the nanoscale has enabled access to materials with extraordinary optical properties, which can interact with biological systems in unprecedented ways, and materials which are able to compartmentalise and release molecular components on demand. In this talk I will show how we have used liposomes, graphene dots and the plasmonic properties of gold nanoparticles to amplify signal for the highly sensitive detection of enzymes and proteins. The translation of these concepts into point of care devices for the diagnosis pancreatitis and rheumatoid arthritis by detection of very low levels of phospholipase A2 will be discussed.

Nature Nanotechnology

Wenjie Sun

Associate Editor, Nature Nanotechnology.

Biography

Wenjie joined Nature Nanotechnology in January 2017, following the completion of her PhD at ETH Zurich, Switzerland. She received her master's degree on colloid and interface chemistry and bachelor's degree on applied chemistry at Shandong University, China. During her PhD at ETH, she focused on the enzyme biochemistry and biophysics within soft matter systems. Wenjie is based in Shanghai.

Abstract

Wenjie will talk about the scope of Nature Nanotechnology, the relationship of Nature Nanotechnology with Nature and other Nature Research journals. And she will share her experience on the editorial process (the workflow and the statistical data) and disclose the criteria of Nature journals from an insider's view. Through the talk, you will know better on what kind of papers a highly selective journal is looking for, how the editors decide whether to send a paper out or not, what they will do when the reviewers' comments are contradictory. And Wenjie is happy to share with you her personal experience as an editor if you are interested and what they are doing to increase fairness and transparency of publishing.

Newcastle – Oral Presentation Abstracts

Solid-electrolyte interphases in Aluminium-ion batteries

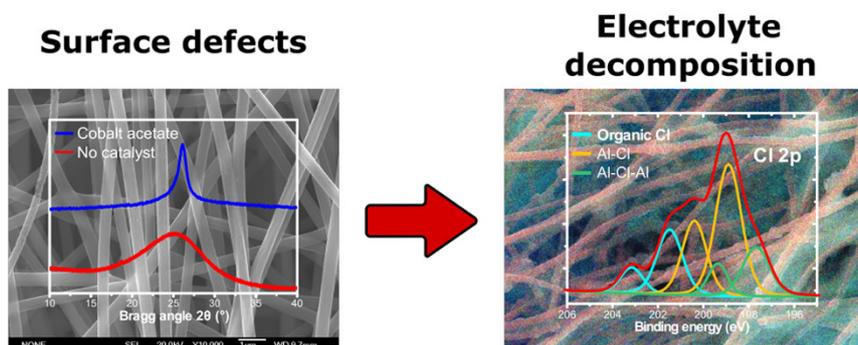
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The recent rise in the worldwide adoption of renewable energy vectors caused an increased demand for large-scale electrochemical energy storage. Current battery technologies such as lithium-ion, however, often lack the cost-effectiveness and safety requirements necessary for large-scale, grid-level energy storage applications. Therefore, it is important to search for alternative technologies, which are more suitable for this purpose. Non-aqueous aluminium-ion batteries (AIBs) are a promising emerging battery technology with several advantages over existing technologies and promising performance.^{1–3}

Currently, one of the most recent challenges in this field involves understanding the phenomenon of poor coulombic efficiency in the first charge-discharge cycle, affecting some types of carbonaceous cathodes.⁴ In this talk, we propose an explanation for this behaviour. By studying the performance of carbon nanofibres with varying degrees of graphitic character, the cause of the poor coulombic efficiency was found to be linked to the formation of a solid-electrolyte interphase, caused by the presence of surface defects in the carbonaceous cathode, promoting the premature decomposition of the electrolyte.⁵



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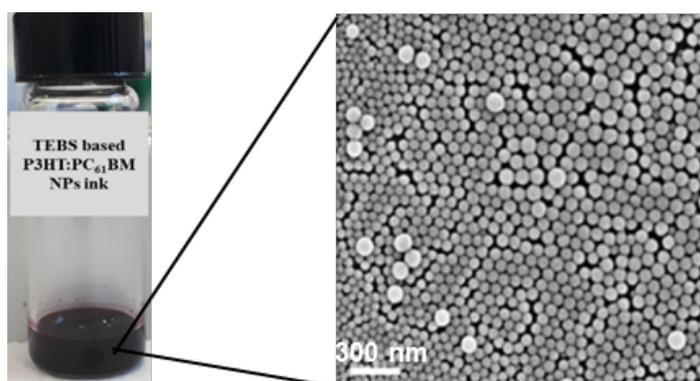
Investigate the morphology of thiophene derivate 2-(3-thienyl) ethyloxybutylsulfonate sodium salt processed aqueous nanoparticles for organic solar cell application

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An eco-friendly aqueous P3HT:PC₆₁BM nanoparticles (NPs) ink has been synthesized using the water soluble thiophene derivate 2-(3-thienyl) ethyloxybutylsulfonate sodium salt (TEBS) surfactant for organic photovoltaic (OPV) device fabrication application. The internal morphology of the nanoparticles as well as their optical characteristics have been investigated using a combination of electron micrograph, UV-vis spectroscopy and x-ray diffraction (XRD) techniques. Most importantly, unlike the core-shell morphology of conventional sodium dodecyl sulphate (SDS) surfactant stabilized NPs, the TEBS NPs form an intermixed donor-acceptor nanodomains revealed by the scanning transmission x-ray microscopy (STXM) composition mapping. Furthermore, a systematic optimization study on TEBS processed NPs size and distribution explores a promising route of this green NPs for OPV (NP-OPV) device fabrication.



Extended electrostatic decay lengths at very high salt concentrations: Examples and Implications

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Many colloidal properties are strongly dependent on the range and strength of Coulomb interactions. In the presence of other ions, the Coulomb interactions between ions are screened such that the interaction energy between charges is exponentially dependent on the separation, this is often expressed in terms of the Debye length.

The surprising observation of long-range electrostatic forces between surfaces immersed in ionic liquids and concentrated salt solutions¹⁻⁵, has recently shown that at high electrolyte concentrations the electrostatic decay length is clearly *not* described by the Debye length and that the electrostatic decay length shows a minimum beyond which the range of electrostatic interactions *increases* with increasing electrolyte concentration.

Several examples of systems that exhibit long-range interactions at high salt concentrations will be presented and the implications discussed.

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Understanding the assembly of amphiphilic additives in bulk and dispersed non-lamellar lipid-based matrices: Phosphorylation, H-bonding and ionisation

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The aqueous channel size of lipidic cubic phases can be a limiting factor for certain applications. For this reason, additives have been used to exquisitely control their nanostructure. In this study, two families of primary phosphoesters have been designed, synthesised and utilised to determine the effect of the positioning of the guest additive at the interface of the host mesophase, and to contrast the effect of headgroup ionisation and protonation.¹ A general methodology has been developed to produce primary phosphoesters, and a unique use of ³¹P-NMR has been used in order to systematically investigate the influence of these additives on monoolein- and phytantriol-based bulk lipidic cubic phases and dispersed cubosomes.

In general, di-phosphorylated additives exhibit a greater effect upon lipid packing than the mono- and tri-phosphorylated molecules due to their optimal positioning (Fig. 1). In dispersion, the protonation state of the phosphate headgroups was manipulated by altering the pH, where shifts in pK_a determined by ³¹P NMR were used as a fluorescent label-free method to identify the location and ionisation state of the phosphate additives. This study systematically evaluates the influence of the positioning of the additive, headgroup size and charge of phosphorylated lipids on the behaviour of lipidic mesophases.

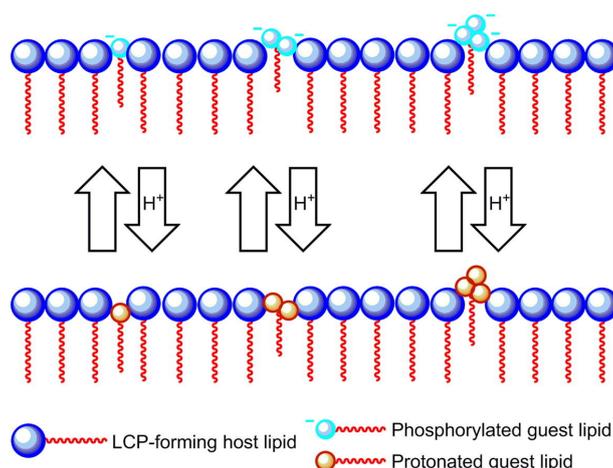


Fig. 1 – schematic demonstrating how ionisation influences the positioning of mono-, di- and tri-phosphorylated lipids at the lipid-water interface in a lipidic cubic phase.

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Extracellular vesicles: Don't hold you breath

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Research in the area of extracellular vesicles have exploded due to their novel biomedical applications, such as disease diagnosis or drug delivery. Extracellular vesicles are defined as nanosized particles with a lipid bilayer and are found in most bodily fluids. Their composition and physical properties are unique to the cell of origin, therefore extracellular vesicles can be used to determine whether a cell is diseased or not. Recently, the Goreham research group reported the isolation and characterisation of breath-derived extracellular vesicles.¹ Extracellular vesicles were isolated from breath condensate and subsequently captured onto a gold substrate using a self-assembled monolayer and an aptamer to target CD63 (a common target protein for extracellular vesicles). Electrochemical impedance spectroscopy measured an increase in resistance upon extracellular vesicle capture and this complimented the results obtained with surface plasmon resonance. This was the first report of the isolation, characterisation and capture of breath-derived extracellular vesicles and offers the first steps to a disease breathalyser.

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Liquid marbles: Particle extraction and transport

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The electrostatic method of liquid marble formation allows contactless delivery of solid particles from a particle bed to a liquid droplet. This process has greatly expanded the variety of structures that can be formed, and the range of potential applications. To fully realise this potential, the process must be precisely controlled, and that requires a detailed understanding of the formation process. Three broad factors influence this process: (1) the morphology and strength of the electric field and the particles' reaction to it (2) the interparticle cohesion and friction forces in the particle bed and (3) the shape of the liquid droplet and the interaction of the particles with the liquid. Each of these three factors is coupled in a complex manner with the other two, and various approaches have been adopted to model them and their couplings. The electric field and electrostatic force on the particles were modelled analytically using an idealised sphere-charged plate model^{1,2}, and more realistically using a finite element model realised in COMSOL Multiphysics. This latter model incorporated gravitational and electrostatic deformation of the droplet, and the resulting adjustment of the field morphology. Extraction of particles from the bed by the electrostatic force was modelled as a stochastic process analogous to the initiation of brittle fracture from micro-cracks³. One fascinating aspect of the interaction of non-conducting particles with the droplet was their mutually-distanced self-arrangement at the liquid/gas interface, possibly the result of lateral dielectrophoretic repulsion.

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‘Dumbbell’ polymer brushes: understanding the origins of non-monotonic structures

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Stimuli responsive polymer brushes offer the ability to modify interfacial properties such as wettability and lubricity as well as control biofouling. Surface-initiated ARGET ATRP has been utilised to synthesise pH and temperature responsive copolymer brushes which were subsequently characterised *in situ* with ellipsometry.^{1,2} Neutron reflectometry (NR) revealed depletion regions in the polymer volume fraction profile (PVFP) near the silicon subphase resulting in ‘dumbbell’ like shaped PVFPs. There is no accepted mechanism through which depletion regions arise in brush conformations.³⁻⁵ Numerical self-consistent field theory was employed to investigate the role segment configuration along the polymer chain has on the conformation of copolymer brushes. Enrichment of charge segments near the interface was found to be responsible for the increased brush hydration in the depletion regions. Understanding the origins of these unusual surface structures is important to develop relationships between surface structure and other interfacial properties.

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Insight into Specific-Ion Effects in Aqueous, Non-Aqueous and Nanostructured Solvents from Quantum Chemical Simulations

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Specific-ion effects and the Hofmeister series have been known since the 1880s. Despite intense research, our understanding of their origins remains poor. We present multiscale quantum chemical simulations that probe how inorganic salts influence the structure and solvency of aqueous and non-aqueous molecular solvents. More complex nanostructured solvents, such as ionic liquids and deep eutectic solvents are also explored. These simulations provide new and fundamental insights into the origins of specific ion effects, for both aqueous and non-aqueous solvents [1,2]. On the basis of quantum chemical energy decomposition analyses, we propose a new mechanism for explaining reversals to the Hofmeister series based on the competing magnitudes of ion-solvent and ion-solute interactions, and their relative Lewis Strengths. We also report a new *ab initio* electrostatic descriptor that explains post-hoc observed specific-ion effects and Hofmeister series in a range of contexts, from polymer cosolvency, enzyme activity and the Gibbs Free Energy of transfer.

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Liquid marbles using electrostatics: effect of particle conductivity, density and shape

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The electrostatic method for liquid marble formation has shown great promise in allowing contactless particle delivery to pendent liquid droplets. However, size has been shown to be a significant limitation in the selection of suitable particles for this transfer process. Here we reduce our previously reported size limitation¹ using conductive copper particles as small as 6 μm diameter, delivering them to a 5 μL pendent water droplet at applied voltages between 0.5 and 3.0 kV.²

The interplay of particle density, conductivity and cohesion have also been studied in relation to the successful formation of liquid marbles.³ Here prior work on monodisperse, spherical latex particles has been expanded by adding thin conductive polymer shells to both these core particles and glass particles of similar size. Conductivity and cohesion have been shown to be competitive interactions with the former enabling and the latter hindering initial particle extraction from a negatively charged packed bed,. Whilst increasing the shell conductivity has previously been seen to facilitate particle extraction, this was not observed for the increased core particle density over the conductivity range studied. This was related to the increase in extraction force required to overcome gravitational forces with high-density particle samples found to more difficult to extract.

Conductive polymer coatings were also successfully applied to hexagonal polyethylene terephthalate platelets for subsequent study as liquid marble stabilisers.⁴ The uncoated and coated platelets were used to form liquid marbles through both the traditional rolling and electrostatic transfer methods of water droplet encapsulation. Substantially different behaviour was observed compared to droplet stabilisation by spherical particles.

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The structure of polymer brushes in complex environments

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Polymer brushes are routinely grown from solid substrates to change surface behaviour to suit particular applications. In many instances these properties, such as wettability, lubricity, adhesion and even anti-fouling, are related to the nanostructure of the brush. We have demonstrated brush structure can be finely tuned by varying solution pH, temperature or salt concentration and identity *independently*.^{1,2} Here, a poly(ethylene glycol) methyl ether methacrylate (POEGMA) copolymer brush was exposed to aqueous solutions containing two electrolytes, where both salts were from the same end of the Hofmeister series or were from either end.^{3,4} The net overall impact of electrolyte addition was found to be dependent on the relative amount of each salt and the system temperature. Copolymer brushes of poly(2-(2-methoxyethoxy) ethyl methacrylate) (PMEO₂MA) and poly(2-(diethylamino)ethyl methacrylate) (PDEA) respond to changes in temperature and pH. When exposed to salt, the effect of each electrolyte on the copolymer brush conformation could be switched by changing the pH from low (charged DEA) to high (uncharged DEA).^{5,6} The overall behaviour of the copolymer in each salt was PDEA-like at low pH, and MEO₂MA-like at high pH.

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Constructing monodisperse polymer micelles based on the concept of Platonic micelle

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It has been theoretically asserted and experimentally proven that the aggregation number (N_{agg}) of spherical micelles is distributed over a range of values, so our knowledge of the thermodynamics of micelle formation suggests that truly monodisperse spherical micelles would not emerge. However, we previously demonstrated that when the N_{agg} of spherical micelles composed of calixarene-based amphiphiles is 20 or less, the structures are discretised and the N_{agg} s are always match the vertex numbers of regular polyhedra, that is, Platonic solids; therefore, these structures are named “Platonic micelles” (Figure 1).¹ We have so far identified many Platonic micelles in the micelle composed of small-molecular surfactants² and a reverse micellar system³. Therefore, we suppose that this concept of Platonic micelle is universal rule for any micellar systems, meaning it would also be applicable for constructing Platonic polymeric micelles.

Controlling the interfacial area (a_e) between hydrophilic domain and hydrophobic domain is required for constructing Platonic micelles. However, it seems to be difficult to control the a_e in the polymer system because of the flexibility of polymer chain conformation which is also affected by the solution condition such as pH, salt concentration, and temperature. In this paper, we employed molecular bottlebrush (MB) structure into the hydrophilic part to solve the problem. The a_e of the MB-based surfactant (MBS) can be systematically controlled using controlled radical polymerization. We evaluated the structure including the morphology and N_{agg} of MBS-based micelles using small angle X-ray scattering, light scattering, and analytical ultracentrifugation measurements, and will discuss it in the presentation.

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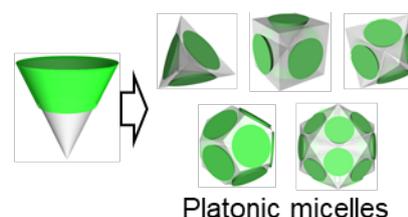


Figure 1. Schematic illustration of Platonic micelles composed of con-shaped surfactants.

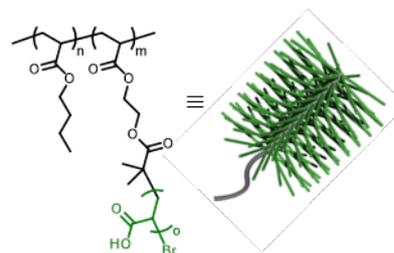


Figure 2. Chemical structure and schematic illustration of molecular bottlebrush-based surfactant.

Hydration Layer Structure of Biofouling Resistant Nanoparticles

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Hydrophilic surface chemistries can strongly bind water to produce surfaces that are highly resistant to protein adsorption and fouling. The interfacial bound water and its unique properties have intrigued researchers for decades yet the relationship between the water three-dimensional structure and function in antifouling coatings remains elusive. Here, we use hydrophilic, epoxy organosilane modified silica nanoparticles to demonstrate cheap, robust and practically applied coatings that we discover have broad-ranging, ultra-low antifouling properties when challenged by various proteins, bacteria and fungal spores. To understand their remarkable antifouling properties, Frequency Modulation-Atomic Force Microscopy is used to directly observe the interfacial water structure on single nanoparticles at sub-atomic resolution (Figure 1), which we validate using all-atom MD simulations that strikingly predict similar structures of water layers on the original and ultra-low fouling surfaces [1]. Unprecedented convergence of experimental and modelling data reveal that suitably spaced, flexible chains with hydrophilic groups interact with water molecules to produce a confluent, *quasi-stable* layer, consisting of dynamic interfacial water, provides an effective basis for antifouling performance of ultrathin, hydrophilic surface chemistries

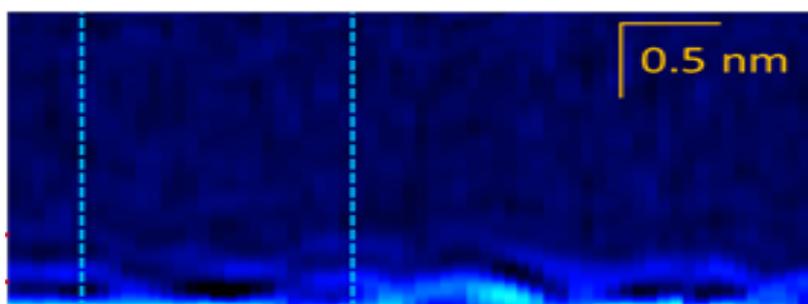


Figure 1: 3D FM-AFM cross-sectional image of interfacial water structure on silica nanoparticle.

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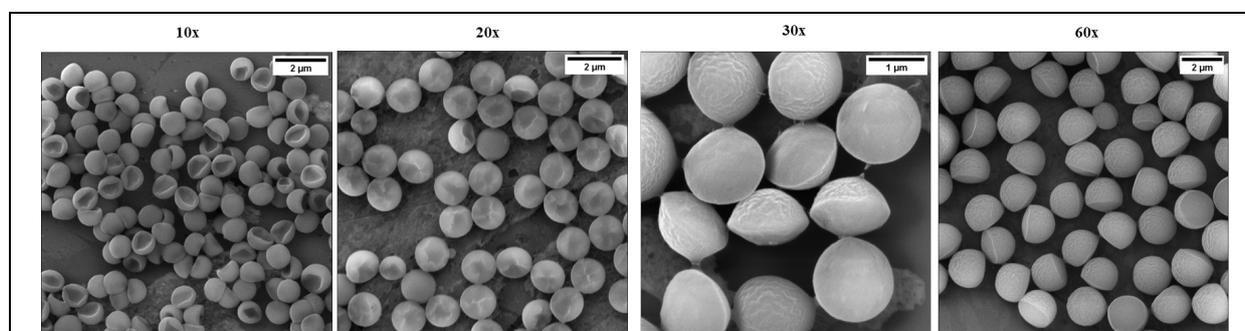
A simple and flexible strategy for the preparation of non-spherical Janus particles

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The preparation of complex colloidal particles, *i.e.*, particles with non-spherical shape and asymmetric functionality, also known as Janus particles, has been the subject of numerous investigations in the literature. In spite of the broad variety of methods proposed over the last two decades, the preparation of Janus particles with controlled size, shape, functionality still remains a burden. The objective of this work is to propose a simple, reproducible and very flexible method to prepare polymer-based colloidal particles in the micron and sub-micron size range, with non-spherical shape and asymmetric functionalization. The method typically starts with simple polystyrene particles as seeds, and is followed by an activated swelling step with dioctanoyl peroxide, as both initiator and activated agent, a technique pioneered by Ugelstad three decades ago. This is followed by a second swelling step, where a variety of monomers (typically acrylates) can be used, and finally by free radical polymerization to consolidate the particles. This type of polymerization, leads to a Janus particles, with polystyrene confined on one part of the particle surface and the acrylates on the other side. When inhibitors are not removed during the second polymerization step, non-spherical particles are obtained, with shapes ranging from dimpled particles, to flattened spheres to diamond-like particles can be easily prepared, as shown in the figure, were particles prepared with different swelling ratios are showcased. In addition of being a highly reproducible synthesis, the particles are size controllable by playing with the seed size and the swelling ratio, easily functionalised by using functional acrylates, and can be easily prepared in very large quantities, making a unique example of how complex colloidal particles can be readily and flexibly synthesized.



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Elasticity as a biomarker for cancer-derived extracellular vesicles

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Cancer cells can be up to 70% softer than their non-malignant counterparts and determining the cancer cell elasticity (how soft or hard a cell is) can be used as a cancer diagnosis tool. All cell types, including cancer cells, are known to release nano-sized vesicles, named extracellular vesicles (EVs), which can function as biomarkers for cancer. EVs are involved in cell-cell communication and are composed of DNA, RNA, and proteins within a phospholipid membrane that is specific to the cell they originate from. Although biomarkers in EVs offers a novel mode of cancer diagnosis, identification of biomarkers has been described as “finding a needle in a haystack”. With that said, there are bulk differences in the physical aspects of EVs such as the stiffness, size and adhesion properties. Atomic force microscopy of these lipid-based vesicles is a versatile technique that can be used to extract relevant physical information such as bending modulus of the lipid membranes, roughness of the surface of the vesicles, elasticity and adhesion. With this project, we aim to determine the elasticity variations between EVs derived from prostate cancer throughout the life-cycle (different degrees of metastasis). Preliminary results of this analysis are shown here with the relation of the different physical properties measured for normal prostate cell line-derived vesicles and the correlation of their adhesion, stiffness and deformation. This analysis will further be extended to probe EVs derived from prostate cancer cells of different metastatic potential. The results will further aid in cancer diagnostics and in improving the understanding of the active involvement of the EVs in cancer development.

Newcastle – Poster Abstracts

Discovery and Development of Drug Delivery Systems for Non-Ideal Active Pharmaceutical Ingredients

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Non-ideal active pharmaceutical ingredients (APIs) represent a significant share of existing pharmaceutical products as well as developing drug leads.^{1,2} Both aqueous solubility and membrane permeability are properties crucial for drug efficacy *in vivo*, as they will affect the degree of drug transport and cell permeation.³ One way to overcome the issue of poor aqueous solubility or membrane permeability amongst non-ideal APIs is the use of drug delivery systems; by encapsulating therapeutic cargo, the drug delivery system will supersede the properties of the drug with its own once in solution.

This PhD seeks to investigate drug interaction with potential drug delivery systems by complementing experimental and computational techniques, with the goal of using this information to discover and develop more effective drug delivery systems. Lipidic lyotropic liquid crystals (LLCs) and cucurbituril (CBn) inclusion complexes have been identified as potential candidates for development. Preliminary results of molecular dynamics simulations demonstrate spontaneous permeation of solubility limited Pitstop® 2 into a DOPC lipid bilayer (**Fig. 1**) when starting in the bulk water phase. By confirming simulations with experimental SAXS/SANS measurements, molecular dynamics can be utilized to give an atomistic resolution of drug position and kinetics in LLCs; something which is much more difficult to measure experimentally. Future work will involve modelling more complex LLCs (**Fig. 2**), as well as using density functional theory (DFT) calculations to assess the interaction of Pitstop® 2 with CBn macrocycles and potential analogues.

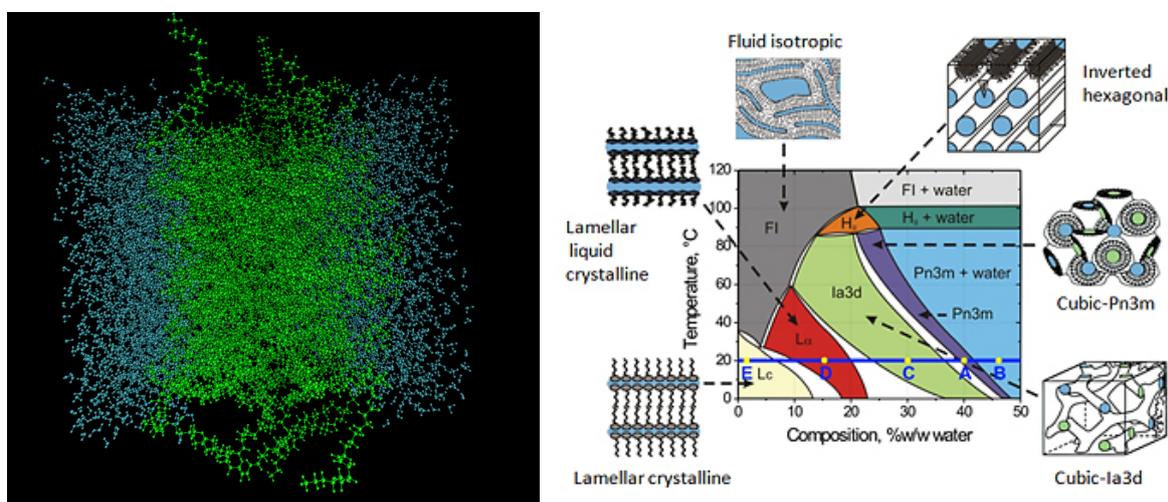


Figure 1 (right) Molecular dynamics simulation of a DOPC bilayer
Figure 2 (left) Phase diagram of monoolein in water

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Investigating the Interactions Between Lipidic Mesophases and the Human Gastrointestinal Microbiome

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This proposal aims to answer three clear questions about the interaction between the surface and internal structure of lipid mesophase particles that are inserted into the gastrointestinal tract, and the complexities of the human microbiome:

1. How does the lipid particle surface and structure influence the microbiome?
2. How does the microbiome influence the surface and structure of particles?
3. Can this mechanism be manipulated to enhance drug and nutrient absorption?

How drugs and nutrients are processed and absorbed by the body is still a poorly understood field of science, which limits the development of life-saving, cost-appropriate medications. This process is complicated by the action of the host's microbiome, which has been shown to metabolise both drugs and nutrients before absorption by the host.^{1,2} Not only is microbial metabolism determined by the specific composition of the microbiota – which is highly variable across time and between individuals – but the drugs and metabolites present in this ecosystem also influence the composition of the microbiota.^{3,4}

Lipid mesophases are promising matrices for drug delivery, offering significant benefits to existing oral formulations. Their biocompatibility, enhancement of drug stability and absorption, and stimuli-responsiveness have led to increasing interest in these nanomaterials. The encapsulation of enterally administered drugs in lipid mesophases is proposed as a method of mitigating complex drug-microbiota interactions. However, the fate of these nanomaterials in the gut is unknown, specifically, the role of the microbiota in this process.

Lipidic mesophases have shown to increase the absorption of actives on-demand, but their application has been limited due to an incomplete understanding of what happens *in vivo*.⁵ In order to make advancements towards better nutrition and treatments, what occurs at the interface between these materials and the action of the microbiome needs to be understood.

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Computational Investigations of Solvent and Ion Structure Containing Dissolved Ions at Varying Concentrations

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The presence of ions in many chemical, biological and physical systems can dramatically change the behaviour of that system¹. A predictive theory of such effects is still elusive and much of this behaviour is ion-specific and not fully explained by a simple metric of the ion such as its size or charge, or by a property of the system such as concentration or dielectric constant². These effects are known as specific ion effects (SIE), and a subset of this is the well-known Hofmeister series³⁻⁵. Observations of SIE are also not restricted to aqueous systems, and the understanding of ions in non-aqueous systems is much less understood^{3,6}.

In this ongoing work, results from molecular dynamics (MD) calculations using the AMOEBA⁷ polarisable force field are presented, examining how different concentrations of ions affect the structure of the solvent, and also how the ions themselves correlate with other ions. Concentrations ranging from 0.01-5m have been investigated, in an attempt to ascertain any discontinuities or irregularities as the solubility limit is approached, including re-entrant behaviour that is observed at high concentrations⁸⁻⁹.

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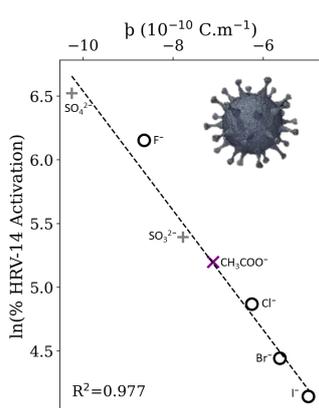
The electrostatic origins of specific-ion effects

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Specific ion effects (SIEs) relevant to the physical, biological, chemical, environmental and material sciences have long gone without a fundamental understanding to their origins, or a subsequent predictive theory.¹ Existing theories are unable to adequately explain and predict frequently-observed series reversals and anomalies.^{2–5} Building on previous work,^{6–7} we establish the physical origin of the Hofmeister series of SIEs to be the dominant electrostatic potential energy (U_E) of ions in the system. A new ion parameter, ρ (“sho”), correlates with SIEs in various water properties, co-nonsolvency effects and enzyme activities. U_E and ρ respectively provide the basis towards new general predictive theories and a tool for describing ion interactions.



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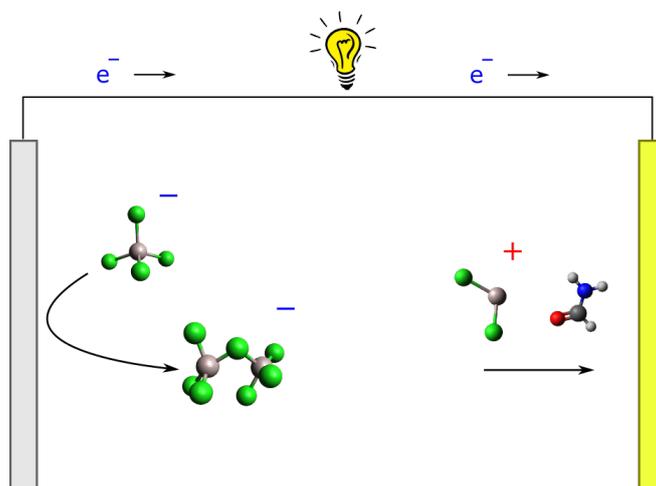
Energy dense Al-ion batteries

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Aluminium batteries have the potential to provide a high capacity while offering greatly reduced costs in comparison to their lithium counterparts due to the over-whelming abundance of aluminium. However, current electrolytes are expensive and thus limit commercial viability. By using aluminium halide salts in a eutectic with a small polar compound, a cheap ionic liquid analogue can be obtained. These eutectic mixes have the added benefit of being less corrosive than the standard ionic liquids used. Herein we present some novel electrolytes with these cheap ionic liquids, as well as some conductive frameworks which provide capacity as well as delivering electrons into the other active material.



Uniform Spacing of Particles on a Pendent Droplet Surface Under the Influence of a Non-Uniform Electric Field.

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During transport to a pendent droplet using an electric field in order to form liquid marbles¹⁻², certain hydrophobic particles have demonstrated a striking uniform spacing on the droplet surface during the initial stages of coating as revealed by video imaging at 180 fps (Figure 1). This phenomenon is exhibited by both conductive and insulating particles as long as they are sufficiently non-wetting. This work aims to elucidate the origin and factors that contribute to this significant interparticle spacing such as electric field strength, particle contact angle and particle conductivity.

To this end, insulating lycopodium spores were surface modified in order to vary particle contact angle. Whilst polypyrrole coated polystyrene of varying sizes (20 – 140 μm diameter) were studied to investigate the impact of particle size on this unusual phenomenon.



Figure 1. 140 μm hydrophobic conductive particles spacing out on a 5 μL pendent droplet under the influence of a non-uniform electric field. Needle diameter is 1.2 mm for scale.

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A novel pathogen sensing platform for detection of *Escherichia Coli* in Water

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Contamination of water by pathogens particularly *Escherichia Coli* (*E. coli*) presents a major challenge to human health today. These outbreaks not only burden healthcare systems but result in major financial and reputational damage to governments and water-treatment industries. The economic cost of managing impacts and plant shutdowns can be avoided by timely detection of the bacteria but most conventional techniques are labour intensive, time consuming and require high pathogen concentrations for effective detection. In this work, we capture and quantify outer membrane vesicles (OMVs) released by *E. coli* cells. As cellular excreta, these vesicles exhibit similar outer membrane proteins, composition and characteristics of the parent bacterial cell and can be used as abundant alternative targets¹ for *E. coli* detection. In doing so, we exploit specific DNA aptamers that selectively bind to the surface of OMVs, while examining their surface interactions and binding affinity to aid sensitive and efficient capture. In conjunction, we develop a dual detection platform that combines impedance based electrical and optical measurements to allow for rapid, robust and cost-effective detection of *E. coli* OMVs in potential industrial applications.



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Specific ion effects on the behaviour of thermoresponsive polymer brushes

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Specific ion effects relate to any phenomena which depend on the identity of ions present in a system, and not merely their valence or concentration. One subset of specific ion effects is the Hofmeister series, which orders ions on their ability to either stabilise (salting-in ions) or destabilise (salting-out ions).¹ In recent years, thermoresponsive polymer brushes have been used as exemplar systems to study specific ion effects.² Thermoresponsive polymer brushes consist of end-grafted polymer chains, which undergo a phase transition from well to poorly solvated over a given temperature range, establishing an interface with switchable physicochemical properties.

The influence of mixed aqueous electrolytes and non-aqueous electrolytes on the behaviour of polymer brushes is limited, as there is no all-inclusive theory regarding specific ion effects. As natural environments are comprised of complex electrolytes, understanding the interplay of different ions in various solvents is imperative for real world applications. The thermoresponse of a poly(oligo(ethylene glycol) methacrylate) (POEGMA) statistical copolymer brush was monitored as a function of temperature in a variety of mixed electrolytes.^{3,4} In the presence of these mixed electrolytes, a non-monotonic concentration-dependent influence of the two anions on the thermoresponse of the brush was observed. The manifestation of two salting-in ions on the behaviour of a POEGMA brush was dependent on the influence of the ions with the polymer chains, whereas the impact of two salting-out ions was dependent on the available solvent molecules. Much can be gained by improving our knowledge of ion specificity and understanding the subtle structural changes of a brush are essential to unravel the dominant drivers behind specific ion effects.

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