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Table of Abstracts

1. Zahra et al. — *MXene-Reinforced Elastomeric Polymer Nanocomposites with Enhanced Electrochemical Energy-Storage Performance*
2. Azeem et al. — *Peptoid-Nanoparticle Conjugates as Synthetic Affinity Probes for Bacterial Interaction Across Strains*
3. Billina et al. — *Probing Small-Molecule Interactions via Magnetic Relaxometry of Engineered Gd^{3+} -Nanoparticle Platforms*
4. Choudhary et al. — *Plasma-Activated Textile Electrodes with Borophene Nanosheets for High-Performance Flexible Supercapacitors*
5. Choudhary et al. — *Sputtering-Engineered WO_3/MnO_2 Multilayers on Graphene for High-Performance Supercapacitors*
6. Coksu et al. — *2-Hydroxypropyl- β -Cyclodextrin-Driven Nano-Self-Assembly of Ethyl 3,4-Dihydroxybenzoate: Enhanced Antioxidant and Anticancer Activity*
7. Devine et al. — *Polymer Based Theranostics for Pancreatic Cancer Therapy*
8. Dunn et al. — *Metallic Nanoplatfoms for Rapid Theranostic Treatment in Pancreatic Cancer*
9. Franchi et al. — *High-Pressure Synthesis and Exfoliation of Layered Sb_xP_{1-x} Nanosheets*
10. Fraser et al. — *Balancing Toxicity and Potency: Active Machine Learning-Guided Discovery of Antimicrobial Peptoids*
11. Futtly et al. — *Engineering Conditional Peptide Self-Assembly Using AlphaFold*
12. Graham et al. — *Nanoscale Precision in the Synthesis of Hybrid Nanomaterials for Remote-Controlled Applications*
13. Hallam Stewart et al. — *A Slippery (Thermal) Slope: Transient Self-Assembly During Heating Controls the Mechanical Properties of Supramolecular Gels*
14. Harris et al. — *Aerosol-Assisted Chemical Vapor Deposition (AACVD) of Transition Metal Dichalcogenides for Catalytic Applications*
15. Harris et al. — *Using AlphaFold2 to Investigate Self-Assembling α -Helical Peptide Structures*
16. John-Pierre et al. — *Particle Size Analysers: Assessing Instrument Accuracy Against Polydisperse Formulations*
17. King et al. — *Maple Syrup as a Natural Electrolyte for Low-Power, Sustainable Organic Transistors*
18. Kontou et al. — *Rational Design of Polymeric Nanoparticles for the Delivery of Biologics for Cancer Therapy*

19. Li et al. — *Development of Biodegradable Molecularly Imprinted Nanoparticles for Specific Recognition of N-Acetylneuraminic Acid*
20. Lopez et al. — *Evaluating Nanoparticle Transport in a Spheroid Co-culture Lung Model*
21. Maurya et al. — *A Design Rule for Stereochemical Encoding of Supramolecular Architecture*
22. Mc Ginley et al. — *Developing the First Covalent Functionalisation Reaction for 2D Borophene Oxide*
23. Nayar et al. — *Graphene Foams as Heterogenous Catalyst Support Materials for the Click Reaction*
24. O'Meara et al. — *Entrapping Gemcitabine Hydrochloride in Solid Lipid Nanoparticles for the Treatment of Pancreatic Cancer*
25. Omoyeni et al. — *Green Phytofabrication of Silver Nanoparticles from Underexplored Cypriot Plant Species with Tunable Antimicrobial, Antioxidant and Anticancer Activity*
26. Rahmatpanah et al. — *Overcoming Ocular Barriers: Polymersome Nanoparticles*
27. Reid et al. — *Size-Controlled Nitrocellulose Nanoparticles and Metal-Biomolecule Nanocomposites for Potential Use in Biosensing and Theranostic Applications*
28. Sanders et al. — *Core@shell Nanoparticles for Stimuli-Responsive Drug Delivery*
29. Seal et al. — *Evaluating Acoustic Wave Propagation in Hydrogel Networks Modified via Peptide-Resin-Mediated In Situ Gold Nanoparticle Nucleation*
30. Shayoub et al. — *Nanoparticle Delivery of Ruthenium Polypyridyl DNA Probes*
31. Sushkova et al. — *Field-Responsive Self-Healing Coatings Based on Magnetic Nanoparticles*
32. Trinidad Torras et al. — *Magnetically Actuated SERS Nanosensors for the Rapid Detection of Contaminants of Emerging Concern in Water*
33. Zakari et al. — *Exploring Prussian Blue Hybrid Nanostructures for Photocatalytic Degradation*

MXene-Reinforced Elastomeric Polymer Nanocomposites with Enhanced Electrochemical Energy-Storage Performance

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Abstract

MXene nanosheets, known for their high strength, electrical conductivity, and efficient ion transport, are promising materials for next-generation energy storage. Herein, SEBS-g-MA/Ti₃C₂T_x nanocomposites were fabricated via solution casting. XRD confirmed the intercalation of MXene layers, while SEM and EDX mapping revealed well-dispersed and strongly adhered MXene nanosheets within the elastomeric matrix. Binder-free electrodes exhibited a high specific capacitance of 375 F g⁻¹, attributed to the conductive layered MXene network and enhanced ion/electron transport. The results demonstrate the potential of SEBS-g-MA/MXene nanocomposites as flexible electrodes for advanced energy-storage applications.

INTRODUCTION

MXene-based polymer composites are being studied for a wide range of applications, including photovoltaic, medicinal, energy storage, and electromagnetic shielding¹. Tuning the conductivity of polymeric materials is being investigated with the addition of conductive nanofillers as, MXene, CNTs etc to the polymer matrix^{2,3}. In this work, incorporation of MXene is reported in variable proportion with respect to specific capacitance while maintaining or barely altering its other original characteristics.

RESULTS & DISCUSSION

By fabricating effective conducting routes, the incorporation of Ti₃C₂T_x MXene changed the insulating SEBS-g-MA polymer into an electrochemically active composite. The proportion of MXene showed an increasing trend

with the charge storage behaviour the magnitude of specific capacitance was improved up to 375 F g⁻¹ with 70% of MXene by weight in SEBS-g-MA/Ti₃C₂T_x nanocomposites

CONCLUSIONS

SEBS-g-MA/Ti₃C₂T_x nanocomposites were successfully fabricated with well-dispersed MXene nanosheets, confirmed via structural and morphological analyses, while binder-free electrodes achieved a high specific capacitance. Increased specific capacitance was attributed to MXene proportion, thus keeping the processibility and elastomeric nature of polymer matrix. The results highlight the potential of these flexible nanocomposites for advanced energy-storage applications.

ACKNOWLEDGEMENTS

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- University of Glasgow, Glasgow, Scotland
- Higher Education Commission Pakistan

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Peptoid-Nanoparticle Conjugates as Synthetic Affinity Probes for Bacterial Interaction Across Strains

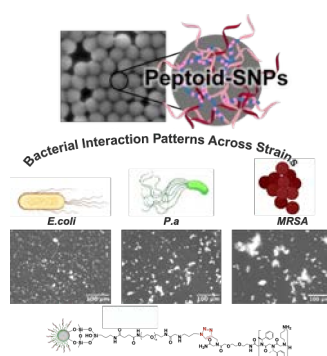
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Abstract:

Antimicrobial resistance (AMR) is a major global health threat, and rapid identification of the infectious agent is key to targeted therapy. Current methods are slow and confined to the laboratory. Peptoids, synthetic peptide mimics with tuneable side chains and resistance to proteolysis, are a promising molecular scaffold for selective bacterial recognition [1]. We developed synthetic affinity probes from silica nanoparticles functionalised with antimicrobial peptoids, and compared the effects of coupling the sequence from different chain ends and the presence or absence of a PEG spacer, the latter of which controls the peptoid distance from the particle surface. The peptoid- and PEG-modified silica nanoparticles were screened against *Escherichia coli*, *Pseudomonas aeruginosa*, and MRSA using optical microscopy. The results corroborated our earlier findings for peptoids coupled on microscopy slides that the attachment parameters generated large effects on the amount of bacteria binding [2]. Further quantitative image analysis showed that the PEG spacer controls surface accessibility for different bacterial strains. Peptoid-only coatings caused aggregation, whereas a PEG spacer restored particle dispersion, and the effect depended on both the coupling direction and the bacterial strain. This is consistent with steric stabilisation that keeps the peptoid probe available for binding. These results support our hypothesis that surface presentation drives strain-specific binding and suggest a route toward label-free biosensing and rapid, point-of-care bacterial identification based on only a small number of antimicrobial binding sequences.



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Probing Small-Molecule Interactions via Magnetic Relaxometry of Engineered Gd³⁺-Nanoparticle Platforms

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Responsive MRI nanoprobes offer a powerful route to non-invasive detection of molecular biomarkers. However, their development is limited by an incomplete understanding of how nanoparticle structure influences analyte interactions. Here, we investigate how nanoparticle architecture modulates the signal response of Gd³⁺-chelates towards molecular analytes through a series of modified silica nanoparticles.

INTRODUCTION

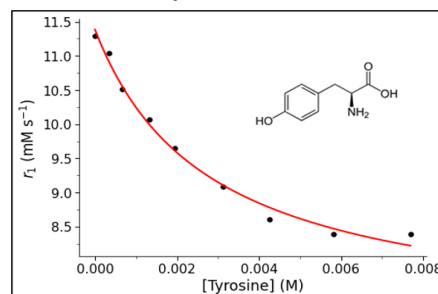
Molecular sensing of biologically relevant analytes is crucial for understanding cellular function, disease progression, and therapeutic response. While traditional modalities like fluorescence spectroscopy offer high sensitivity, its application *in vivo* is constrained by limited tissue penetration, photobleaching, and interference from complex biological matrices. Comparatively, magnetic resonance (MR)-based sensing provides non-invasive, quantitative detection of analyte interactions deep within tissues.¹

Nanoparticlebased MR-probes have emerged as promising sensing platforms due to their tuneable structures and improved signal over conventional smallmolecule Gd³⁺-based contrast agents.² While significant advances in the design of responsive small-molecule MR-probes have been achieved, extending these principles to nanoparticle-based systems remains a challenge due to an incomplete understanding of how nanoparticle structure influences sensing mechanisms.³ Consequently, the mechanistic basis of analyte-responsive signal modulation in nanostructured systems is poorly defined, limiting their wider application.

RESULTS & DISCUSSION

Here we present a series of silica nanoparticles functionalised with a Gd³⁺-DOTA-silane species and systematically varied architectures to investigate the influence of nanoparticle structure on analyteresponsive relaxivity. In addition to enhanced signal over their molecular counterparts, the probes are highly sensitive to their local environments, displaying measurable MR-signal upon addition of biologically relevant analytes (Figure 1). By varying factors such as porosity and functionalisation location we demonstrate how analyte-responsive signal can be tuned with nanoparticle structure.

Figure 1. Relaxivity response of Gd³⁺-doped nanoprobes to the amino acid tyrosine at 25 °C, 1.5 T.



CONCLUSIONS

Gd³⁺-doped nanoprobes exhibit improved signal over their molecular analogues and are highly responsive to their local environments. Control over nanoparticle architecture offers a promising route towards the rational design of highperformance nanoprobes for small-molecule detection and diagnostics.

ACKNOWLEDGEMENTS

Our thanks are extended to the University of Birmingham and EPSRC for funding.

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Plasma-Activated Textile Electrodes with Borophene Nanosheets for High Performance Flexible Supercapacitors

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Abstract

The rapid advancement of smart power technologies requires flexible, lightweight, and highperformance energy storage systems. In this work, borophene-modified silver cloth electrodes are developed as a promising platform for flexible supercapacitor applications. Borophene, an emerging two-dimensional boron-based material, possesses high electrical conductivity, a large accessible surface area, and favourable surface chemistry, making it attractive for rapid charge storage and efficient ion/electron transport.

Pristine Ag cloth was selected as a flexible and conductive current collector. Before active material deposition, the Ag cloth was activated using oxygen plasma treatment to enhance surface wettability, generate active surface sites, and improve adhesion between the textile substrate and borophene nanosheets. Borophene was subsequently synthesized, dispersed, and deposited onto the plasma-treated Ag cloth through a coating process. Different borophene weight percentages were investigated to optimise active material loading, electrode uniformity, ion diffusion pathways, and electrical conductivity.

The fabricated electrodes were characterized using FTIR, XRD, RAMAN, SEM, and TEM to examine functional groups, crystallinity, structural features, and nanosheet morphology. Electrochemical performance was evaluated using Gamry workstation CV, GCD, and EIS to analyse good capacitive behaviour, resistance, charge–discharge response and cycling retention for the flexible supercapacitor device.

Keywords

Borophene; Silver Cloth; Oxygen Plasma Treatment; Flexible Electrode; Supercapacitor; Electrochemical Energy Storage.

Sputtering-Engineered WO₃/MnO₂ Multilayers on Graphene for High Performance Supercapacitors

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Abstract

Hybrid material strategies provide an effective approach for integrating the advantages of carbon-based materials and transition metal oxides, thereby simultaneously enhancing the power and energy densities of supercapacitors. In this study, a flexible composite electrode was fabricated by depositing multilayer WO₃/MnO₂ thin films onto a graphene substrate via combined DC and RF magnetron sputtering techniques. The optimized four-layer-by-layer (4 LBL) architecture demonstrated improved electrical conductivity, abundant electroactive sites, and shortened ion/electron transport pathways. In addition, life cycle assessment (LCA) of the electrode provided insight into its environmental sustainability, supporting the development of a high-performance electrode with enhanced electrochemical behaviour and long-term cycling stability.

Consequently, the 4 LBL@graphene electrode exhibits a high specific capacitance of 494.2 F g⁻¹ at 5 mV s⁻¹ and excellent rate performance. A symmetric SC device based on this electrode operates steadily within 0.8 V, delivering a specific energy of 44 Wh kg⁻¹ at a specific power of 521 W g⁻¹ and retaining 89% of its initial capacitance after 10,000 cycles at 10 A g⁻¹. The device also demonstrates outstanding flexibility and low internal resistance (2.40 Ω), highlighting the strong potential of 4 LBL@graphene for next-generation flexible energy storage applications.

Keywords

Energy Storage, Supercapacitor, DC and RF Magnetron Sputtering, Multilayer, Symmetric Device.

2-Hydroxypropyl- β -Cyclodextrin-Driven Nano-Self-Assembly of Ethyl 3,4Dihydroxybenzoate: Enhanced Antioxidant and Anticancer Activity

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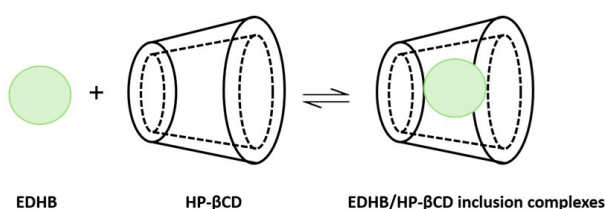
Abstract

Ethyl 3,4-dihydroxybenzoate (EDHB) is a poorly water-soluble phenolic compound with promising biological activities. Its limited aqueous solubility limits its bioavailability and therapeutic potential [2]. This study aimed to improve EDHB biological performance through HP- β CD complexation. EDHB/HP- β CD inclusion complexes were prepared by solvent evaporation and characterized using phase-solubility analysis, molecular docking, structural, morphological, and thermal analyses. HP- β CD enabled nanoscale self-assembly with particle sizes below 200 nm. The complex exhibited antioxidant activity and distinct cell-dependent oxidative responses. Moreover, HP- β CD complexation enhanced EDHB cytotoxicity against MCF-7 and MDA-MB-231 cells, particularly MCF-7, while showing favorable biocompatibility in L929 cells. These findings highlight HP β CD-driven nanoself-assembly as an effective approach for enhancing EDHB bioactivity.

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Figure 1. Schematic illustration of EDHB/HP β CD inclusion complex formation.



Preferred Format: Poster

Polymer Based Theranostics for Pancreatic Cancer Therapy

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Abstract

By integrating metallic nanoparticles into a polymeric nanoparticle delivery system, we aim to combine two proven nano-delivery techniques to harness key aspects of both. Enhanced delivery and biocompatibility from the polymer will be coupled with the imaging capabilities associated with the metallic core. This ultimately will result in improved efficacy of current treatment options as well as accelerated diagnosis and staging. Initial work will develop the synthetic conditions required to combine these two technologies with further work planned to produce a continuous manufacturing pipeline. In-vitro and In-vivo studies will later hope to confirm the safety and efficacy of the final delivery system.

INTRODUCTION

Pancreatic cancer represents one of the most bleak forms of the disease. Late diagnosis, poor treatment efficacy and difficult morphology all contribute to the abysmal 5-year survival rate of just 13%.¹

Current treatment options are highly limited and have remained largely stagnant for decades. Surgical resection is the only curative treatment however only 20% of cases are resectable upon diagnosis.¹ The current first line non-surgical treatment is the combination chemotherapy regimen FOLFIRINOX which suffers from severe side effects and low patient response.²

Diagnosis is another challenging aspect with 48% of patients displaying distant metastasis at the point of diagnosis. This can be attributed to late presenting, easily misinterpreted symptoms and poor imaging methods which carry significant misdiagnosis risk.^{1,3}

RESULTS & DISCUSSION

Both the amphiphilic polymer⁴ and the hybrid metallic nanoparticle⁵ have established synthetic routes. Building on a database of existing data, an

optimised system for the inclusion of the metallic moiety within the polymer structure will be developed.

Once the combined system has been developed, analytical testing will confirm the validity of the process and look to assess the chemical and physical properties.

Further work aims to address the lack of feasible scale up for nanoparticle-based therapeutics by investigating the potential of micro/milli-fluidic manufacturing techniques rather than current batch processes. Again, building upon previous research in this area.⁶

CONCLUSIONS

By building on existing knowledge around the diagnosis and treatment of Pancreatic cancer, using nanotechnology, we aim to produce a combined theranostic tool to improve the outlook of patients by enhancing therapeutic efficacy and enabling faster and more effective diagnosis.

ACKNOWLEDGEMENTS

Thank you to EPSRC centre for doctoral training in cyber-physical systems for medicines development and manufacturing (CEDAR) for funding this work.

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Preferred format: Poster

Presentation Title

Metallic nanoplatforms for rapid theranostic treatment in pancreatic cancer

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ABSTRACT

Multifunctional nanotechnology offers great potential in the diagnosis and treatment of disease. Pancreatic cancer (PC) comes with grim prognosis; thus, improved treatment is crucial. Gold-iron oxide hybrid nanoparticles (HNPs) utilise iron oxide nanoparticles (IONPs) in diagnostic imaging, and gold nanoparticles (AuNPs) in photothermal therapy (PTT) – allowing for earlier diagnosis and expedited treatment. This work aims to explore the impact of continuous manufacture on the synthesis of HNPs for use in PC diagnosis and treatment. The efficacy of HNPs as a multifunctional nanotechnology will be tested in-vitro and in-vivo, if results prove favourable, in PC models.

INTRODUCTION

A major factor contributing pancreatic cancers ~ 13 % 5-year survival is late diagnosis, where symptoms are non-specific and usually only present following metastasis.

Iron oxide nanoparticles (IONPs) improves clarity of diagnostic imaging, acting as a contrast agent in magnetic resonance imaging.² IONPs accumulate at the PC site, if present, creating a darkened region allowing for earlier, more confident diagnosis.

Gold nanoparticles (AuNPs) exhibit localised surface plasmon resonance (LSPR) when irradiated with near-infrared wavelengths, a phenomenon which produces specific, localised heating. Thus, AuNPs can be used to thermally ablate cancerous cells without harming surrounding healthy tissue.

HNPs utilise both nanotechnologies to diagnose *and* treat PC (theranostics).³ Accumulation PC site can be visualised using the IONP core and treated immediately by PTT using the AuNP shell. HNPs may also be functionalised with drug, for targeted treatment by controlled drug release.

RESULTS & DISCUSSION

HNPs are initially synthesised by a well-established synthetic route.^{3,4} IONP core is synthesised via coprecipitation of Fe₃O₄, reacting dissolved iron sulfate in sulphuric acid with sodium hydroxide and potassium nitrate. IONPs are then magnetically washed and resuspended in water. AuNPs are synthesised by reduction of chloroauric acid with sodium carbonate and sodium borohydride.

HNPs are coated in alternating polyethylene imine and AuNPs via electrostatic interactions. A coating of polyethylene glycol is added to improve biocompatibility, followed by a final gold shell by direct reduction of chloroauric acid with hydroxylamine onto HNP surface.

Various analytical techniques will be utilised at each synthetic stage to study synthesis and coating stages (e.g. dynamic light scattering, ultravioletvisible spectroscopy, Fourier-transform infrared spectroscopy, transmission electron microscopy).

CONCLUSIONS

HNP characterisation should see increasing diameter with each coating stage and alternating positive and negative surface charge per polymer and AuNP coating, respectively. Success of each coating will be quantified, and surface morphology will be investigated.

ACKNOWLEDGEMENTS

Thank you to EPSRC centre for doctoral training in cyber-physical systems for medicines development and manufacturing (CEDAR) for funding this work.

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Preferred Format: Oral

High-Pressure Synthesis and Exfoliation of Layered $\text{Sb}_x\text{P}_{1-x}$ Nanosheets

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Group 15 nanomaterials such as two-dimensional P, As, Sb and Bi sheets, and one-dimensional P nanoribbons (PNRs) possess a wide range of attractive properties, including high carrier mobilities and highly tunable band gaps across a wide energy range.^{1–3} While pristine materials have been proposed for numerous applications

(optoelectronics, thermoelectric, water splitting) alloying has emerged as a powerful strategy for accessing additional functionality.^{4–6} Versus PNRs, AsP nanoribbons possess enhanced electron mobility and a narrowed bandgap,⁷ however, beyond AsP, phosphorus-pnictogen alloys remain largely unexplored.

We examine the system SbP; amorphous $\text{Sb}_x\text{P}_{1-x}$ precursors were synthesized at a range of composition ratios via a salt metathesis reaction and crystallized by application of high pressure and temperature in a multi-anvil apparatus, finding them to adopt the puckered, van der

Waals structure of β -Sb. Further, these materials has been successfully exfoliated to afford novel, highly crystalline SbP nanosheets (Figure 1). Establishing SbP as a new layered group 15 alloy provides a promising platform for extending the

compositional and electronic tunability of twodimensional pnictogen materials.

ACKNOWLEDGEMENTS

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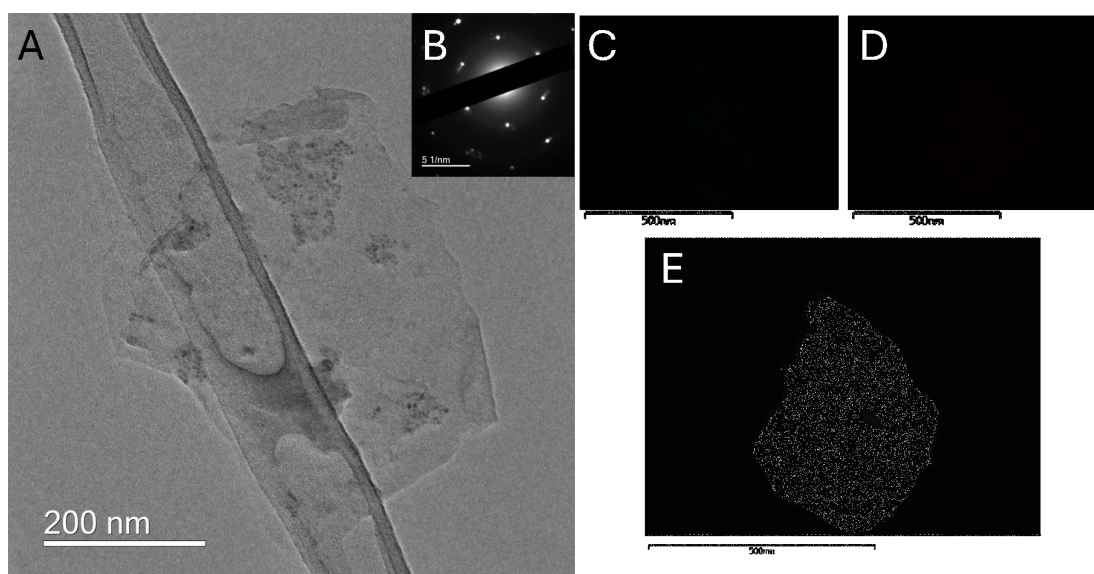


Figure 1 – (A) TEM image of SbP nanosheet supported by lacey carbon grid; (B) SAED collected at site of TEM image; EDS maps of Sb (C) and P (D) content across SbP flake; (E) darkfield STEM image of SbP flake

Preferred Format: I'm happy with Oral or Poster

Balancing Toxicity and Potency: Active Machine Learning–Guided Discovery of Antimicrobial Peptoids

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ABSTRACT

To tackle antimicrobial resistance (AMR), novel antimicrobial compounds must be developed.^{1,2} Inspiration was taken from natural antimicrobial peptides (AMP) and expanded upon using peptoids. The compounds were simulated using Martini³ and GROMACS coarse-grained molecular dynamics (CGMD) simulations. A new metric was developed to measure potency and cytotoxicity in a single metric, $\Delta\Delta$ -area per lipid ($\Delta\Delta$ APL). Property-aware design rules were then developed, and new AMP candidates were identified based on machine learning $\Delta\Delta$ APL predictions. The results were validated by *in vitro* minimum inhibitory concentration (MIC) measurements for several sequences.

INTRODUCTION

As bacteria are rapidly evolving AMR, novel antimicrobials are urgently needed.^{1,2} AMR has a higher likelihood of developing against antimicrobials which have specific binding targets, making methods like membrane disruption more appealing. This kills the bacteria through membrane-breaking mechanisms such as forming holes. As this method does not rely on specific binding targets, the bacteria would require large cellular changes to evolve AMR. AMPs are a natural solution to this problem and have been effective for millions of years. To further improve on AMPs, peptoids are instead used as they provide numerous benefits such as higher stability and chemical diversity.⁴

RESULTS & DISCUSSION

The CGMD simulations identified peptoids with high potency against bacterial bilayers (75:25

POPE:POPG) while exhibiting low potency against mammalian bilayers (60:40 POPC:CHOL). This was captured by the $\Delta\Delta$ APL, allowing $\Delta\Delta$ APL to be used as a target for identifying high potency, but low toxicity AMPs. Therefore, leveraging machine learning and $\Delta\Delta$ APL, new promising AMPs were identified, and electrotopological state was determined to be the main feature leading to a high $\Delta\Delta$ APL.

CONCLUSIONS

In conclusion, the use of $\Delta\Delta$ APL metric as a combined measure of both cytotoxicity and potency shows strong potential for bilayer differentiation in a single metric. By using $\Delta\Delta$ APL as the target for machine learning algorithms, the model was able to predict possible hit compounds and suggest structural properties that could be altered to further increase the $\Delta\Delta$ APL result.

ACKNOWLEDGEMENTS

This work was supported by the Nature Inspired Acoustics CDT – Funded by The Leverhulme Trust

All simulation results were obtained using the ARCHIE-WeSt High-performance Computer (www.archie-west.ac.uk) based at the University of Strathclyde

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Preferred Format: Poster

Engineering Conditional Peptide Self-Assembly Using AlphaFold

Helen Fiddy^{*a}, Sofia Chinelli^{a,b}, Ravi R. Sonani^c, Tomás S. Plivelic^d, Annela Seddon^e, Edward H. Egelman^c,
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Abstract.

Programming self-assembly from peptide sequence remains difficult because existing design rules are only weakly predictive of emergent supramolecular behaviour. Here, we show that AlphaFold Multimer can be used to engineer conditional peptide self-assembly by simultaneously selecting for co-assembly and against assembly of the individual components. Using model confidence metrics as proxies for assembly propensity, we designed peptide pairs that largely remain unstructured in isolation, but form defined tape-like nanostructures upon mixing. Experimental measurements including circular dichroism, small-angle X-ray scattering and cryo-electron microscopy validate the predicted behaviour across multiple systems. These results establish artificial intelligence-guided design as a practical route to programmable supramolecular peptide materials.

INTRODUCTION

Self-assembling peptides make up an excellent class of supramolecular materials due to the inherent tuneability of the amino acid sequence. Despite this, there is a surprising lack of diversity in existing self-assembling peptide systems. AlphaFold Multimer¹⁻³ has been shown to predict short peptide assemblies with varying degrees of success. We hypothesized that we could use AlphaFold as a design tool to predict both assembly and non-assembly of two-component peptide systems⁴.

RESULTS & DISCUSSION

Through an AlphaFold guided rational design approach, we established a set of ground rules with which to approach predictions of short peptides. Using local confidence metrics as a proxy for self-assembly, we designed several co-assembling peptide systems. We used techniques such as circular dichroism, small angle X-ray scattering, and

cryo-electron microscopy to experimentally verify the predicted structures. We show that AlphaFold can distinguish significant behavioural changes between subtly different systems.

CONCLUSIONS

To conclude, we show that we can use an AlphaFold guided rational design approach to design two-component co-assembling systems. Using AlphaFold confidence metrics as guidance, we designed multiple peptide pairs with subtle differences in amino acid sequence. AlphaFold can distinguish between their behaviour despite their similarities.

ACKNOWLEDGEMENTS

Work in the EHE lab was supported by NIH GM122510. We thank the University of Virginia's Molecular Electron Microscopy Core (supported by NIH grants G20-RR31199, SIG S10-RR025067 and U24-GM116790) for its support in cryo-EM experiments. The Ganesha X-ray scattering apparatus used for this research was purchased under EPSRC Grant "Atoms to Applications" (EP/K035746/1). We acknowledge the MAX IV Laboratory for beamtime on the CoSAXS beamline under proposal 20241517.

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Nanoscale precision in the synthesis of hybrid nanomaterials for remote-controlled applications

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This presentation will discuss AuNP/UiO-66 hybrid nanomaterials assembled using chemospecific dynamic covalent linkages. Post synthetic assembly of hybrid AuNP/UiO-66 nanomaterials allows for individual tuning of the size and stoichiometry of the AuNP and MOF building blocks. To exploit the size-dependent photothermal properties of the AuNP component, we first developed a systematic approach for tuning the size of AuNPs bearing reactive ligand shells. This approach has enabled the construction of AuNP/UiO-66 hybrids with size control over the AuNP component. We are now investigating the size-dependent photothermal effect in porous plasmonic hybrids for applications in cargo release and catalysis.

INTRODUCTION

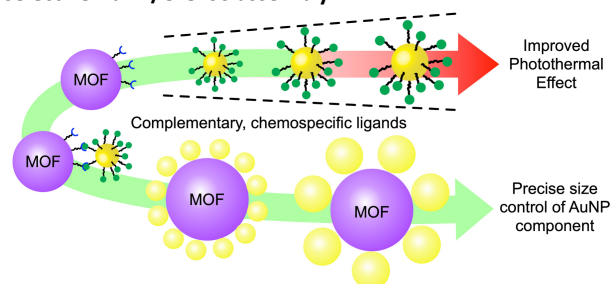
Gold nanoparticles (AuNPs) are an attractive component for 'hybrid' nanomaterials owing to their distinct chemical and optical properties, which can be tuned by choice of nanoparticle size, shape, and surface chemistry.¹ The advent of reliable methods for the preparation of nanometre-sized metal-organic framework (MOF) particles now raises the prospect of incorporating their readily tunable properties and huge internal surface areas into nanostructured assemblages and materials.² We have shown that dynamic covalent links can be used to assemble hybrid nanomaterials from reaction-enabled AuNP and MOF(UiO-66)-NP building blocks. Chemospecific dynamic interparticle linking allows for independent control over the structure of each nanoparticle while ensuring intimate mixing of the nanoscale building blocks with readily tunable stoichiometry.³ We now aim to create hybrid

AuNP/UiO-66 nanomaterials that exploit sizedependent photothermal properties of AuNPs.

RESULTS & DISCUSSION

Size-selective synthesis of AuNPs bearing a reactive ligand monolayer is non-trivial. We have developed a systematic workflow and automation tools that apply Hansen Solubility Parameters (HSPs) to characterize nanoparticle solvation characteristics and, hence, systematically optimise reaction solvent. This workflow has allowed for fine control over the core size of AuNPs bearing reactive ligand monolayers capable of molecule-directed construction of hybrid materials. These building blocks were subsequently used to construct hybrid AuNP/UiO-66 nanomaterials with precise control of the size of the AuNP components. Fine-tuning the photothermal properties of these materials will enable remote control over MOF-based functionality such as catalysis or cargo delivery.

Figure 1. Precise control of AuNP core size enables size selective AuNP/UiO-66 assembly.



ACKNOWLEDGEMENTS

We thank the University of St Andrews, EPSRC and the U.S. Army Research Office (W911NF-20-10233) for financial support. We would also like to thank Dr. Aaron Naden for help with TEM and Jeremy Graham for help with Python.

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Preferred Format: Oral

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A Slippery (Thermal) Slope: Transient Self-Assembly During Heating Controls the Mechanical Properties of Supramolecular Gels

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Abstract.

Heating and cooling is an effective method for preparing supramolecular hydrogels from low molecular weight gelators (LMWGs). Here, we demonstrate the importance of both heating and cooling rates to control the properties of the final gel. These are surprisingly overlooked parameters, but can lead to gels with very different properties.

INTRODUCTION

Peptide-based LMWGs self-assemble into onedimensional nanostructures which entangle to trap water in interstitial spaces, forming a hydrogel. As supramolecular materials, their structure in the nanoscale, as well as the macroscale, is governed by non-covalent interactions. Due to their weak nature, small changes in conditions such as pH or temperature can lead to vast differences in material properties. Thermal history is a widely used but little understood gelation method.

RESULTS & DISCUSSION

Fmoc-phenylalanine (FmocF) is a widely studied LMWG as it is inexpensive, commercially available and has wide application scope in areas such as drug delivery and antibacterial materials.¹ Hydrogels can be formed by heating and cooling low concentration aqueous suspensions of FmocF.² Here, we demonstrate that the thermal pathway contains an unexpected transient self-assembled state that develops during heating and controls the properties of the final gel. Using simultaneous rheology and time-resolved small-angle X-ray scattering (SAXS), we directly follow the structural and mechanical evolution

throughout the entire heat-cool cycle. We show that self-assembly begins during heating, producing a weak, large-scale network that subsequently reorganises during cooling before becoming mechanically locked into the final gel (Figure 1).

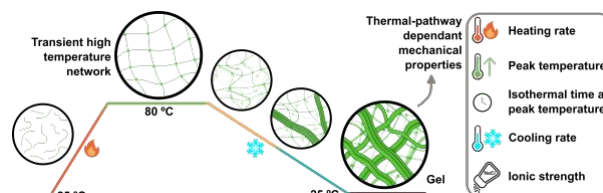


Figure 1. Proposed self-assembly pathway of FmocF heat/cooled hydrogels through time-resolved small-angle X-ray scattering and time sweep rheology.

By controlling the heating rate, cooling rate and thermal hold time, the lifetime and evolution of this transient state can be manipulated, leading to substantial changes in the final mechanical properties. These data demonstrate that thermal history controls gel properties by directing the dynamic self-assembly pathway rather than simply determining the initial and final states.

CONCLUSIONS

By manipulating the self-assembly and subsequent reorganisation of this transient high-temperature network through the thermal gelation pathway, we control the final mechanical properties. Ionic strength is an additional tuning factor, which influences primary nanostructure resulting in changes on the network-scale.

ACKNOWLEDGEMENTS We thank Tenovus Scotland for funding.

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Aerosol-assisted chemical vapor deposition (AACVD) of transition metal dichalcogenides for catalytic applications

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Abstract. This presentation explores the first syntheses of WSe₂ and MoSe₂ via AACVD verified using XRD, Raman, SEM, and XPS. It shows the impact of optimising the precursor solution and AACVD parameters to deposit the desired coating. The potential of the WSe₂ and MoSe₂ coatings as photocatalysts for pollution degradation is demonstrated using methylene blue/crystal violet.

INTRODUCTION

Transition metal chalcogenides (TMDCs) have been of interest in recent years because of their varying and tunable properties.¹ TMDCs are layered nanomaterials consisting of a transition metal and a chalcogen and when reduced to a single layer an indirect to direct band gap transition occurs enhancing catalytic properties as light absorption is improved.² To enhance effective catalyst surface area, a variety of synthetic methods can be used, one being aerosol assisted chemical vapour deposition (AACVD). AACVD utilises the formation of an aerosol of a non-volatile precursor solution. It has the ability to produce uniform high surface area, thin coatings.³ AACVD has been successful at producing other TMDCs such as MoS₂,⁴ but the diselenides have proven elusive.

RESULTS & DISCUSSION

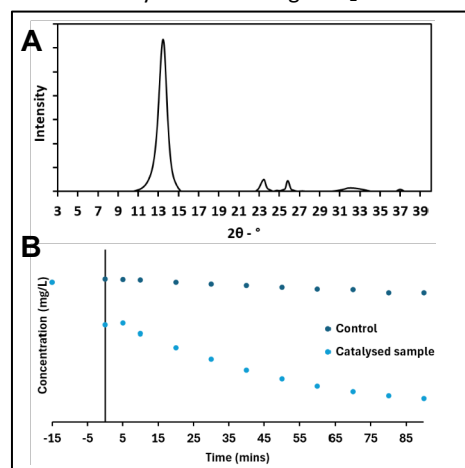
Figure 1A shows the XRD analysis of WSe₂ deposited via AACVD. The peak at 13° indicates the presence of WSe₂,⁵ and the peaks at 23°, 26°, and 32° indicate WO_x.⁵ Figure 1B shows the concentration of methylene blue over 90 minutes with and without the WSe₂ coating present. The WSe₂ degrades the methylene by 85%.

CONCLUSIONS

Both WSe₂ and MoSe₂ coatings were successfully synthesised via AACVD for the first time.

Parameters within the AACVD technique were explored to improve the deposition of WSe₂ and MoSe₂. These coatings were able to photocatalytically degrade methylene blue/crystal violet by ~85%.

Figure 1. (A) XRD analysis of WSe₂ deposited via AACVD; (B) Degradation of methylene blue using WSe₂.



ACKNOWLEDGEMENTS

This work was supported by the EPSRC DTP with Aston University, grant number EP/W524566/1.

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Preferred Format: Oral

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Preferred Format: Oral

Using AlphaFold2 to investigate self-assembling α -helical peptide structures

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ABSTRACT

This research delves into the structural prediction model AlphaFold2, and its potential in *de novo* peptide design. Using AlphaFold2, we aimed to produce α -helical peptides that self-assemble into tape-like coiled structures.

Four α -helical peptides were synthesised using solid phase peptide synthesis, based on the AlphaFold2 predictions. Circular dichroism (CD) spectroscopy was used to decipher α -helical secondary structures. Finally, self-assembling capabilities were defined by small angle X-ray scattering (SAXS) and cryogenic electron microscopy (cryo-EM).

Overall, the structure of the phenylalanine containing peptide within its hydrophobic core, demonstrated the highest degree of similarity to the predicted local distance difference test (pLDDT) and the predicted aligned error (PAE) score of AlphaFold2.

INTRODUCTION

Much research has arisen in self-assembling peptides due to their unfavourable health associations¹. As such, understanding structural behaviours of these peptides is vital for both medicine, and advancements in material science.

Combining known α -helical characteristics with protein prediction models, will enable the fasttracking of *de novo* self-assembling peptides by removing labour intensive lab-based investigations.

RESULTS & DISCUSSION

Peptides 1, 3 and 4 differentiated by the amino acids isoleucine, valine and phenylalanine respectfully, within their hydrophobic core. Peptide 2 on the other hand, housed glutamine in the 1st and 5th positions and tyrosine in the 17th sequence position. Based on AlphaFold2's score satisfaction, each peptide was synthesised at 0.1 mmol, purity levels above 95%, and dissolved in H₂O at 2 mM. The CD spectrum of each peptide had negative peaks at 208

nm and 222 nm found in α -helical structures. SAXS and cryo-EM were also conducted; (Figure 1).

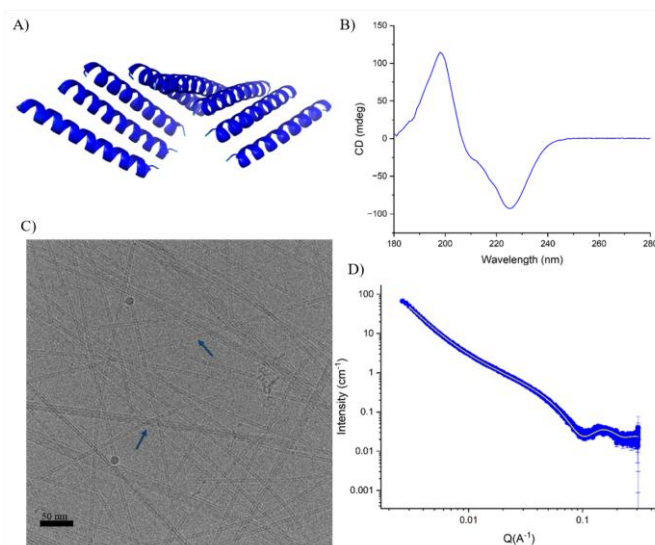


Figure 1. AlphaFold2 predictions of peptide 8 produced using PyMOL² shown at A) The CD spectra, cryo-EM and SAXS are shown at B), C), and D) respectfully of peptide 8.

CONCLUSIONS

AlphaFold2 predicted tape-like structures with nanotube potential upon hierarchical self-assembly of peptides 1, 3, and 4 regardless of hydrophobic residue. The cryo-EM images suggested that only peptide 4 had mirrored the AlphaFold2 predictions. The cryo-EM also aligned with the 1D SAXS data, fitted to a hollow cylinder power law.

To conclude, we aimed to expand the use of AlphaFold2 as an efficient tool in peptide structural predictions. As such, we have shown AlphaFold2 can be an effective design tool in assembling peptides.

ACKNOWLEDGEMENTS

I wish to thank Dr Andy Smith for all his help and insight at the Diamond Light Source.

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Preferred Format: Poster

Particle size analysers: Assessing instrument accuracy against polydisperse formulations

Lois John-Pierre^{*a}, Yvonne Perrie^a

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ABSTRACT (100 word limit)

An investigation was conducted comparing 3 particle sizing techniques i.e. Video Intensity SpatioTemporal Analysis (VISTA), Single-Angle Dynamic Light Scattering (SADLS) and Multi-angle Dynamic Light Scattering (MADLS) to determine the influence of large lipid nanoparticle (LNP) populations on measurement readings to ascertain instrument accuracy, tested at varied dilutions. Preliminary investigations between SADLS & MADLS demonstrated clear identification of larger LNP populations unidentified via SADLS, with VISTA identifying overall smaller populations with higher polydispersity. Current investigation into Single-particle tracking analysis is underway to compare additional particle sizing techniques, as well as reference particle sizing to establish instrument accuracy and solid theoretical ground.

INTRODUCTION

Dynamic light scattering (DLS) is regarded as one of the gold standards of nanoparticle characterization & quality analysis, sizing particles and determining polydispersity index (PDI) efficiently. However, the commonly used SADLS is subject to factors such as intensity bias [1] and form factor [2], which can greatly influence readings of particle size at the nanoscale, leading to inaccurate size measurements and unidentified large populations.

RESULTS & DISCUSSION

The Zetasizer Ultra Malvern Panalytical was used for MADLS and SADLS analyses, with the Lumero Dyneval particle analyser assessing LNP formulations using VISTA. MADLS identified larger LNP populations using a front scattering angle of 11.56°, that were unidentified by SADLS using a scattering angle of 175.2°. VISTA, which uses a statistical physics algorithm to identify populations instead of light scattering, identified smaller and larger LNP populations with an overall greater polydispersity.

CONCLUSIONS

An underestimation of LNP size using DLS particle sizing instruments was determined due to exclusion of larger LNP populations in polydisperse formulations.

ACKNOWLEDGEMENTS

The authors would like to thank the CMAC EPSRC Centre for Doctoral Training in Cyber-Physical Systems for Medicines Development and Manufacturing (CEDAR) (Grant Ref. EP/Y035593/1) for funding this work.

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Preferred Format: Oral Maple syrup as a natural electrolyte for low-power, sustainable organic transistors

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Abstract: We demonstrate the first example of maple syrup-gated organic field-effect transistors as an alternative to synthetic electrolytes for low-voltage transistors. Maple-gated OFETs with p-type P3HT and n-type F₁₆CuPc are compared with identical devices gated with honey, a widely used electrolyte in electrolyte-gated field effect transistors (EGFETs). In both architectures, Maple-gated OFETs demonstrate an improvement of 25% in transconductance (g_m) and a decrease in subthreshold slope compared to honey, demonstrating its potential to be integrated as a material in the next generation of low-power, sustainable electronic systems.

INTRODUCTION

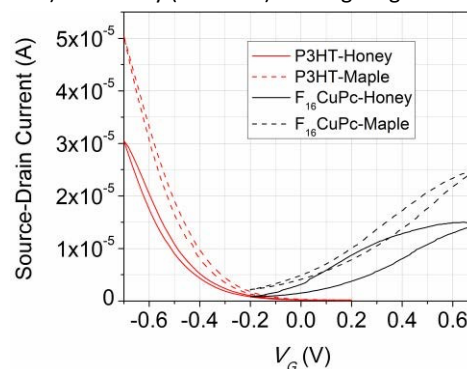
EGFETs, which use an electrolyte as a gating material instead of a polymer or metal oxide, enable electronics with millivolt operating voltages.¹ While synthetic electrolytes have been reported, including ionic liquids, gels, and polyelectrolytes,² the development of sustainable materials for these systems has accelerated, motivated by the need to reduce electronic waste.³ Natural electrolytes such as honey,⁴ which is abundant, low-cost and safe for ingestion, have been reported and could enable the next generation of EGFETs for sustainable electronic systems. Maple syrup, which contains similar ionic species to honey, with lower viscosity and different optical properties, has not yet been explored as a gating material in EGFETs. In this work, we report the first maple syrup-gated EGFETs and compare them to identical honey EGFETs, using p- and n-type semiconductors, to demonstrate the suitability of maple syrup as a gating material in electronic systems

RESULTS & DISCUSSION

Characteristic transfer curves for maple syrup and honey-gated EGFETs in a top-gate bottom-contact architecture are shown in **Figure 1**. The use of maple syrup results in an increase in saturation

current by up to 60%, from 30 μ A to 50 μ A in P3HT devices and from 15 μ A to 25 μ A in F₁₆CuPc devices. The g_m of maple syrup-gated transistors in both cases are up to 25% higher than in honey-gated transistors, increasing from $1.41 \times 10^{-4} \mu$ S to $2.19 \times 10^{-4} \mu$ S in P3HT devices, and from $0.35 \times 10^{-4} \mu$ S to $0.44 \times 10^{-4} \mu$ S in F₁₆CuPc devices. This increase in current and g_m is partially attributed to the capacitance magnitude of maple syrup near DC being approximately twice as high as honey, at 0.36 μ F compared to 0.16 μ F.

Figure 1. Characteristic transfer curves ($|V_{DS}| = 0.7V$) for P3HT (red lines) and F₁₆CuPc EGFETs (black line) using maple syrup (dashed line) and honey (solid line) as the gating material.



CONCLUSIONS

We demonstrate that maple syrup is competitive with honey as a natural electrolyte for low-power EGFETs, yielding mV operation in P3HT and F₁₆CuPc devices, and a 25% improvement in g_m compared to identical devices fabricated with honey.

ACKNOWLEDGEMENTS

This work was supported by a Leverhulme Trust Early Career Research Fellowship (B. K.), and the UKRI Building the Green Economy Theme under UKRI240 (REACT).

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Preferred Format: Poster Rational Design of Polymeric Nanoparticles for the Delivery of Biologics for Cancer Therapy

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Takeda Pharmaceuticals; ^c AstraZeneca.

Abstract. Nanoparticles can be used to increase the solubility of hydrophobic drugs. Polymeric nanoparticles (PNPs) can act as both a drug delivery system and targeting agent due to their ease of surface functionalisation. A four-factor, two-level factorial Design of Experiment has been produced to optimise the formulation of a cationic graft polymer (poly(allylamine)-graft-cholesterol formate) (PAA-g-Chol) for targeted drug delivery for pancreatic cancer. Factors considered in the design include solvent ratios, grafting time, reaction equilibration time, and temperature. System responses included product yield, CAC and critical quality attributes such as particle size, PDI and surface charge (zeta potential).

INTRODUCTION

Cancer medications are inherently insoluble, which hinders their administration to patients and is a major drawback in cancer therapy. This issue currently extends throughout the pharmaceutical industry with more and more new drugs being classed as insoluble. The toxic side-effects inflicted on the body upon administration increases discomfort and pain from a patient care perspective. Materials on the nano scale exhibit unique characteristics, arising from their larger surface area to volume ratio. Nanoparticles can be used to increase the solubility of hydrophobic drugs. Polymeric nanoparticles (PNPs) can act as both a drug delivery systems and targeting agent due to their ease of surface functionalisation. Within this research we aim to optimise the formulation of a cationic graft polymer (poly(allylamine)-graft-cholesterol formate) (PAAg-Chol) for targeted drug delivery for pancreatic cancer.

RESULTS & DISCUSSION

FTIR and ¹H NMR showed successful cholesterol formate grafting with the appearance of carbonyl group stretching at ~1,700 cm⁻¹ for FTIR and the presence of distinct proton peaks in the NMR arising from the aromatic groups present in the cholesterol. CHNOs analysis confirmed that a 5% molar grafting of cholesterol formate was achieved. CAC was reached at 0.1 mg mL⁻¹ PAA-gChol in water. The loading of propofol resulted in micellar swelling with sizes ranging from 200 to 1000 nm, depending on polymer concentration and amount of drug loaded. Regarding the DoE, preliminary results showed no variation in product yield. Analysis of critical quality attributes is ongoing. Full analysis of the factorial design responses, including ANOVA, will identify significant factors, factor interactions and quadratic effects.

CONCLUSIONS

The increase in polymer concentration results in an increase in nanoparticle size when loaded with propofol. The process parameters influencing a polymeric grafting synthesis were evaluated using a DoE approach guided by QbD principles. This study aims to identify the effects of process parameter variation on product yield and critical quality attributes.

ACKNOWLEDGEMENTS

This work was supported by the UK Engineering and Physical Sciences Research Council (EPSRC), Centre for Doctoral Training in Cyber-Physical Systems for Medicines Development and Manufacturing (CEDAR) (Grant Ref. EP/Y035593/1).

Development of Biodegradable Molecularly Imprinted Nanoparticles for Specific Recognition of N-Acetylneuraminic Acid Yining Li, Shu Li, Yi Ge*.

Molecularly imprinted polymers offer highly selective molecular recognition, excellent physicochemical stability and low production costs [1]. However, the poor degradability of conventional MIPs may cause prolonged accumulation in biological systems, limiting their biomedical applications [2]. In this study, biodegradable molecularly imprinted nanoparticles were developed for the selective recognition of N-acetylneuraminic acid (Neu5Ac), a cancer-associated sialic acid biomarker. Molecular docking and quantum-chemical calculations were used to screen functional monomers and optimise the template–monomer pre-polymerisation complex. The nanoparticles were synthesised by precipitation polymerisation using N-isopropylacrylamide, acrylamide and N-hydroxyethyl acrylamide, together with a lactose-based biodegradable crosslinker. The resulting nanoparticles were characterised by FT-IR spectroscopy, dynamic light scattering, binding, selectivity and degradation studies. The MIP nanoparticles exhibited nanoscale dimensions and markedly stronger Neu5Ac binding than the corresponding non-imprinted nanoparticles. They also demonstrated preferential recognition of Neu5Ac over structurally related glucose and N-acetylmannosamine. Moreover, the nanoparticles showed controlled, pH-dependent degradation, confirming the effectiveness of the biodegradable crosslinking strategy. These findings highlight their potential as a multifunctional platform for targeted drug delivery, biosensing and bioimaging [3].

Keywords: molecularly imprinted nanoparticles; Neu5Ac; biodegradable polymers; targeted drug delivery

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Preferred Format: Poster Evaluating Nanoparticle Transport in a Spheroid Co-culture Lung Model

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^a Cell Screening Laboratory, School of Biology and Environmental Science, University College Dublin, maeva.lopez@ucdconnect.ie ^b School of Chemistry, University College Dublin

Abstract. Nanoparticles (NPs) are emerging as attractive vehicles for the delivery of therapeutics in a more targeted manner. NPs are predominantly trafficked to the lysosomes after internalisation, which results in their degradation. This work utilises two biodegradable NP materials, poly(lactic-co-glycolic) acid (PLGA) and Silica (SiO₂), to examine the ability of surface peptide conjugation to alter cellular fate after internalisation. RITC-encapsulated SiO₂ NPs and Rhodamine B-conjugated PLGA NPs were synthesised and their transport in a solid spheroid structure was examined.

INTRODUCTION

Despite there being over 50 approved NP formulations for clinical use, there is still a lack of understanding regarding their interactions with cells and the trafficking pathways they follow once inside. NPs are highly diverse materials which can be readily functionalised for a variety of different purposes and composed of many different organic and inorganic materials. In this work, we have synthesised Rhodamine B-labelled PLGA nanoparticles of ~50-60 nm in size using the nanoprecipitation method. This is a polymer-based nanoparticle with low cytotoxicity that is approved for clinical use¹. Another material with biomedical applications is SiO₂. SiO₂ nanoparticles present several advantages due to their adaptable nature which enables the production of several NP sizes, ease of surface modification and internal encapsulation of materials such as fluorescent dyes.

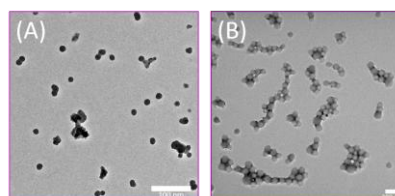
This work is looking at the trafficking of both of these nanoparticle types in complex 3D cellular models known as spheroids. 3D cell models maintain certain aspects of tissue architecture such as cell-cell interactions, cell-matrix interactions, and increased cell type complexity². Nanoparticle transport was examined in a solid spheroid

composed lung epithelial cells and fibroblasts. This is used to assess nanoparticle penetration in a solid tissue.

RESULTS & DISCUSSION

SiO₂-RITC nanoparticles were synthesised using an adapted Stöber method to produce nanoparticles of 73nm in size (Fig. 1a). The nanoparticles showed peak absorbance at 561 nm and peak emission at 580 nm with good dispersibility in water. PLGA nanoparticles were synthesised using the nanoprecipitation method to produce dyeconjugated nanoparticles of 60 nm in size (Fig. 1b). The uptake of these nanoparticles in cells was examined in a solid spheroid model composed of lung epithelial cells and fibroblasts.

Figure 1. SiO₂-RITC (a) and PLGA-Rhodamine B (b) nanoparticles imaged using TEM.



CONCLUSIONS

Unmodified SiO₂ and PLGA nanoparticles show low penetration into a solid spheroid composed of lung epithelial cells and fibroblasts.

ACKNOWLEDGEMENTS

I would like to thank my supervisors and all the members of the JCS and Quinn groups for their help, advice, and training

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A Design Rule for Stereochemical Encoding of Supramolecular Architecture

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Abstract

Understanding how molecular packing controls supramolecular structure is key to the design of peptide-based materials. We hypothesised that local epimerisation disrupts packing within the hydrophobic core, generating packing frustration that promotes lateral protofilament association. By epimerizing phenylalanine residues across the FEFEFKFK sequence, we systematically altered nanostructure radius and morphology. Cryogenic Electron Microscopy (Cryo-EM) revealed transitions from narrow fibrils to wider fibrils, hollow nanotubes, and bundled architectures with increasing radius. These findings demonstrate that chirality of the hydrophobic residue is a key design parameter for tuning supramolecular architecture and the mechanical properties of peptide-based soft materials.

Introduction

Ionic-complementary peptides are promising due to their alternating charged and hydrophobic residues that enhance β -sheet formation and fibrillar assembly¹. While peptide length, hydrophobicity, and charge distribution are well studied, the effects of local stereochemical changes are not. We previously examined how a single Dphenylalanine affects the self-assembly of FEFEFKFK². Now we created various nanostructures by manipulating the chirality of hydrophobic residue in the FEFEFKFK sequence, demonstrating that the position of a stereochemical modification controls fibril dimensions and higher-order organization.

Result and Discussion

To investigate the influence of positional epimerisation for self-assembly and mechanical properties, gels were prepared

from the parent peptide FEFEFKFK and four epimerised analogues (fFEFEFKFK, FEfFEFKFK, FEFEfFKFK and FEFEFKfK).

Cryo-EM was employed to examine how these local stereochemical modifications affected assembly at larger length scales. As shown in Figure 1, all peptides formed long anisotropic nanostructures. The images suggest that radial expansion occurs through the progressive lateral association of protofilaments, leading to increasingly wider assemblies from Figure 1a to 1d. Hence, position-specific epimerisation controls both fibril dimensions and supramolecular morphology rather than simply perturbing an otherwise conserved structure.

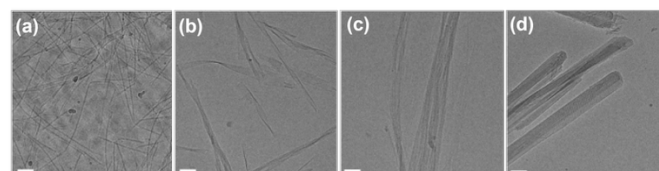


Figure 1. (a) — (d) Cryo-EM images for octapeptides; (a) FEFEFKFK; (b) fFEFEFKFK; (c) FEfFEFKFK; (d) FEFEFKfK

Conclusion

The positional epimerisation within octapeptide sequence serves as a powerful design parameter for controlling hierarchical assembly in the octapeptide sequence of the supramolecular materials.

Acknowledgements: We thank Dr. Diego Alba Venero (ISIS Neutron and Muon Source, Didcot, UK) for help in collecting the SANS data at ZOOM under beamtime allocations. We also thank Dr. Dipankar Ghosh (University of Glasgow) for assistance in data collection under SANS experiments.

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Developing the First Covalent Functionalisation Reaction for 2D Borophene Oxide:

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Abstract:

Borophene oxide (BO), a van der Waals layered crystal of stacked $\sim\text{B}_4\text{O}_3$ layers with potassium cation interlayers, is a promising 2D nanomaterial due to its optical and electronic properties,^{1–3} including high carrier mobility. Grown by a simple ambient oxidation of potassium borohydride (KBH_4) in acetonitrile (MeCN), BO spontaneously dissolves as 2D monolayers (2D BO) in solvents including water, short-chain alcohols, amidic solvents and dimethyl sulfoxide (DMSO), greatly improving the material's processability when compared to traditional 2D nanomaterials while avoiding the defects and intractable phases which are typically required to create stable nanomaterial dispersions.

In this work, we utilise the intrinsic solubility and assumed boronic acid ($\text{B}(\text{OH})_2$) terminal groups of 2D BO in order to covalently modify the nanosheets using the well-established boronate ester diol condensation reaction. This reaction shows high levels of functionalisation ($\leq 10\%$), while being tolerant to both electron withdrawing and donating groups and retaining high crystallinity after the reaction. Additionally, the properties of 2D BO can be modified through these functionalisation reactions, while surface groups introduced by this reaction can be further modified without disrupting the underlying covalent BO network. This work shows the potential of 2D BO as a chemically flexible and easily modifiable nanomaterial of the future for integration into a wide range of devices including sensors, photovoltaics, catalysts and energy storage devices.

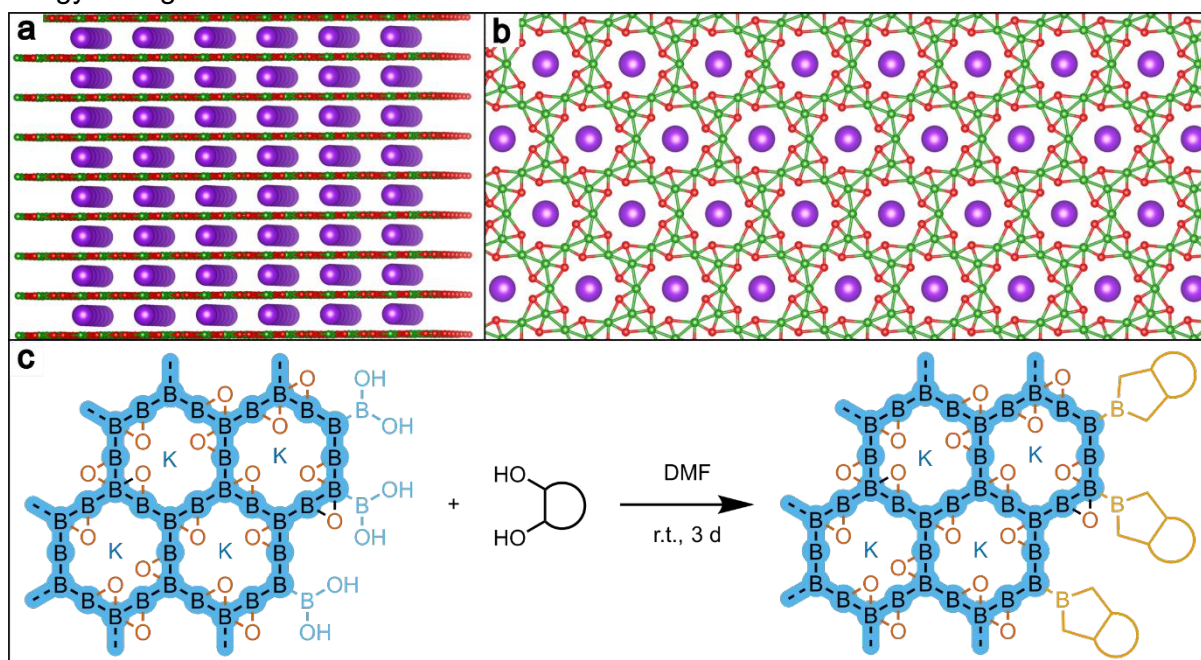


Figure 1: A - Layered crystal and B - in-layer structure of borophene oxide (BO).¹ C - Proposed reaction scheme for functionalisation of BO by boronate ester condensation

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Graphene Foams as Heterogenous Catalyst Support Materials for the Click Reaction

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Abstract. Reduced graphene oxide (rGO) foams with good mechanical properties were produced. A systematic comparison of gas and wet phase precursor deposition methods revealed that wet chemical impregnation of foams yielded unreliable weight loadings and particle sizes compared to gas phase deposition. Commercially available sublimable complexes with the highest and lowest adsorption energies were identified using CREST/GFN2-xTB. This effectively linked the complexes adsorption energies and the leaching of immobilized catalysts. Their catalytic activity was also shown to be better than copper nanoparticles on graphene foams, despite leaching more.

INTRODUCTION

Graphene foams are highly porous 3D structures which possess high thermal stability, electrical conductivity, and surface area.¹ Their open architecture enables efficient mass transport, particularly for flow applications. Copper catalysts can be immobilised as nanoparticles (NPs) or molecular complexes: NPs offer stability, while complexes often show higher activity. Understanding how functionalisation method and catalyst–support interactions affect activity and leaching is therefore essential. Often strongly adsorbing molecular catalysts have large aromatic ligands, on complexes which are not known to sublime.²

RESULTS & DISCUSSION

Here rGO hydrogels made through a hydrothermal method, which were converted to rGO foams through freeze drying and thermal treatments. Copper as introduced via wet- and gas-phase deposition of molecular Cu precursors, followed by flash thermal treatments to convert precursors into NP. Gas-

phase precursor deposition gave higher, more reproducible metal loadings and smaller particles (~80nm) than wet-phase methods (~183nm), which also caused foam contraction and reduced reproducibility. Commercial sublimable copper complexes were screened computationally using a cost-effective semi-empirical method (CREST/GFN2-xTB) to evaluate their adsorption energies on graphitic surfaces. Complexes spanning weak to strong adsorption were identified. In a Cu-catalysed click reaction, computational adsorption energies were correlated with the experimentally observed leaching: strongly adsorbed complexes showed reduced leaching, while weaker ones leached more. In terms of reactivity, immobilised complexes achieved higher yields (~95–98%) than CuNP@rGO (~40%), whereas NP showed lower leaching, demonstrating a trade-off between activity and stability.

CONCLUSIONS

Gas-phase deposition offers improved control over NP formation compared to wet-phase methods. Computational screening effectively predicted catalyst leaching trends. Overall, deposition method, and adsorption energetics govern catalytic performance, providing design principles for heterogenous graphene-based catalysts in future flow applications.

ACKNOWLEDGEMENTS

High performance computing facilities at the University of Leeds. Molecules to Product CDT (grant reference no. EP/L015218/1).

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Preferred Format: Poster

Presentation Title: Entrapping Gemcitabine Hydrochloride in Solid Lipid Nanoparticles for the Treatment of Pancreatic Cancer

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AAbstract.

Pancreatic cancer remains one of the deadliest malignancies, highlighting the need for improved therapeutic delivery systems. This study investigates solid lipid nanoparticles as carriers for pancreatic cancer therapeutics. SLNs were formulated using hot emulsification-ultrasonication, with lipid, surfactant, and cosurfactant compositions varied to optimise formulation characteristics. Particle size, polydispersity index, zeta potential, and entrapment efficiency were evaluated. Formulations achieved particle sizes as low as 87.13 nm with good monodispersity, demonstrating the potential of SLNs for drug delivery. Moderate success was achieved in encapsulating gemcitabine hydrochloride; however, further optimisation is required to improve entrapment efficiency before stability and drug release studies can be undertaken.

INTRODUCTION

Pancreatic cancer (PC) remains one of the most lethal malignancies worldwide with a dismal 5-year survival rate compared to other common cancers (~12%) and is projected to become second leading cancer death by 2030.^{1,2} Solid lipid nanoparticles (SLNs), a second-generation lipid-based nanoparticles offer advantages including solubilisation of hydrophobic drugs, reduced toxicity, controlled drug release, and targeted delivery.⁴ All of which offer significant advantages over conventional therapeutic treatment, such as chemotherapy.

RESULTS & DISCUSSION

Formulation of SLNs was carried out by hot emulsification-ultrasonication varying lipids, surfactants, cosurfactants in a prescreening to determine the optimal formulation with characterisation involving particle size, polydispersity index, zeta potential and entrapment efficiency. Adjusting these parameters has produced particle sizes ranging from as small as 87.13 nm, with corresponding impacts on formulation stability. To date, moderate success has been achieved in encapsulating gemcitabine hydrochloride, a hydrophilic drug.

CONCLUSIONS

In conclusion, SLNs offer great potential in encapsulating drugs, with great particle size and monodispersity. However more work is required in successfully entrapping gemcitabine hydrochloride before finding an optimal formulation to continue stability and drug release studies.

ACKNOWLEDGEMENTS

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Green Phytofabrication of Silver Nanoparticles from Underexplored Cypriot Plants species with Tunable Antimicrobial, Antioxidant and Anticancer activity

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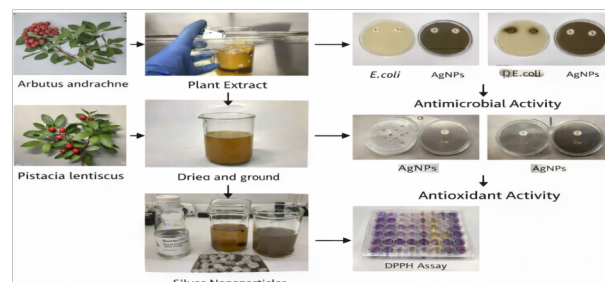
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Abstract INTRODUCTION

Nanotechnology involves synthesizing, characterizing, and using nanostructured related materials for diverse applications. This nanomaterials possess at least one dimension in the nanoscale range (approximately 1–100 nm)¹. At this scale, nanostructured materials exhibit distinct physicochemical properties that differ significantly from their bulk counterparts. Chemical stability and biocompatibility of produced nanoparticle from plant extracts demonstrate medicinal implications, rendering them suitable candidates for antibacterial and antioxidant activities².

RESULTS & DISCUSSION

This study presents the green synthesis of very stable silver nanoparticles from *Arbutus andrachne* and *Pistacia lentiscus* leaf measuring around 90.87 nm and 78.26 nm respectively. The synthesized silver nanoparticles (AgNPs) was characterized using UV-visible spectroscopy, Fourier transform infrared spectroscopy, X-ray diffraction, energy dispersive X-ray spectroscopy, and scanning electron microscopy. Gas chromatography-mass spectrometry analysis was conducted to separate and detect the chemical components of the plants. Their antioxidant, antibacterial and anticancer properties were also examined which makes them suitable for various biomedical applications.



CONCLUSIONS

The green-synthesized silver nanoparticles exhibited potent antioxidant, antibacterial, and anticancer activities, highlighting their potential for a wide range of biomedical applications.

ACKNOWLEDGEMENTS

The authors acknowledge the support and research facilities provided by the Department of Bioengineering research center, Cyprus International University, Nicosia, Northern Cyprus.

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Preferred Format: Oral

Overcoming ocular barriers: Polymersome nanoparticles

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Abstract.

Glaucoma causes irreversible blindness via elevating intraocular pressure (IOP). To overcome invasive injection limitations, we synthesised selfassembling amphiphilic random copolymers integrating polyethylene glycol methacrylate (PEGMA) with hydrophobic long-chain methacrylate. These polymersome nanoparticles exhibited controlled nanostructures with a narrow polydispersity index, providing a versatile platform for targeted intraocular drug delivery. Evaluated using microRNA-29 (miR-29) mimics as a model anti-fibrotic payload, the nanocarriers yielded a 4fold increase in cellular uptake in corneal and TM lines in vitro. Ex vivo bovine assays showed enhanced matrix mobility (7.0 mm/hr vs 1.7 mm/hr for free drug), demonstrating robust tissue penetration for topical therapy.

INTRODUCTION

Glaucoma is a leading cause of vision loss, driven by TM extracellular matrix fibrotic remodelling that elevates IOP. Current treatments for posterior eye pathology require invasive intravitreal injections, as effective non-invasive topical delivery remains an unmet clinical challenge. Polymersome nanoparticles—self-assembled vesicular structures with tuneable membrane chemistry—offer a versatile platform to protect therapeutic molecules and facilitate transcorneal transport. These nanocarriers enable topical delivery of diverse therapeutics, including microRNA-29 (miR-29) mimics as a model anti-fibrotic strategy. Here, we synthesised amphiphilic random copolymers to engineer polymersome nanocarriers for non-

invasive ocular drug delivery.¹

RESULTS & DISCUSSION

Designed polymersome nanoparticles were constructed from amphiphilic random copolymers synthesised with a fixed 5:3 hydrophilic-tohydrophobic monomer ratio, combining PEGMA (500 Mn), decyl methacrylate (C10), cholesteryl methacrylate, and cationic monomers. Selfassembled via reverse-phase evaporation, these polymersomes formed uniform nanostructures with narrow size distributions (100–300 nm) and low polydispersity (PDI < 0.5), facilitating robust electrostatic complexation with miR-29 mimics. As an advanced delivery platform, the polymersomes achieved a 4-fold enhancement in cellular uptake across human corneal epithelial (HCE) and TM cell lines compared to unformulated payloads. Furthermore, ex vivo bovine organ culture models confirmed superior matrix mobility and tissue penetration for the fluorescently tagged polymersomes, reaching a vitreous transport rate of 7.0 mm/hr versus 1.7 mm/hr for the free drug.

CONCLUSIONS

Designed polymersome nanoparticles offer a noninvasive topical delivery platform that overcomes ocular barriers and delivers therapeutics to target tissues for glaucoma treatment.

ACKNOWLEDGEMENTS

This research was generously funded by Invest Northern Ireland.

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Preferred Format: Poster

Size-Controlled Nitrocellulose Nanoparticles and Metal-Biomolecule Nanocomposites for Potential Use in Biosensing and Theranostic Applications

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ABSTRACT

This study presents a combination of previously unreported advances in the production and use of nitrocellulose particles. These include the controlled, tunable synthesis of nitrocellulose particles (mean diameter of 52 nm); the production of Ag and Au nitrocellulose nanocomposites; the retention of a biologically active protein (fluoroBSA), and attachment of a T4 bacteriophage. Bound phage retained notable antimicrobial activity after air-drying and storage, whilst free phage had none. These novel metal-biomolecule nanocomposites are potentially a platform for biosensing and many theranostic applications.

INTRODUCTION

To address several life-threatening conditions, such as cancer, sepsis, and antimicrobial-resistant infections, the scientific community has recently focused on developing all-in-one theranostic methods for rapid, specific detection and treatment of diseased cells^{1,2}. To investigate their applicability to address these issues, the controlled synthesis of nitrocellulose particles was performed. The production of metal nanocomposites and the completion of retention and functionality assays for the biomolecules (proteins and viruses) were also investigated.

RESULTS & DISCUSSION

Nitrocellulose particles, tuned between 52 and 500 nm, were synthesised using an adapted bottom-up synthesis method³, pH 8 buffer (optimised from the tested 6–12 pH range), 10 min post-stirring time (after nucleation), and a colloidal suspension at 20°C. Zeta sizing, Nanoparticle Tracking Analysis, and Scanning Electron Microscopy (SEM) were used to determine mean particle sizes. Nanocomposites were produced by adding Au and

Ag nanoparticles to the synthesis suspension (prenucleation), with implementation concentration verified by UV-Vis and SEM imaging. Ag nanoparticles were noted to be more diffuse throughout the nanocomposite, Au mostly aggregating and not incorporated. The binding of test protein (fluoroBSA) to the Ag nanocomposite particle surface was confirmed by fluorescence imaging. The T4 phage (at a concentration of 1.7×10^8 pfu mL⁻¹ in PBS) had a mean binding of 89% (n=6); however, only 8% were bound in a plaqueforming orientation on the 500 nm particle surface. The correctly orientated bound phage remained biologically active against its target bacterium, *Escherichia coli*. Early indications suggest that rehydrated bound phage remained active after airdrying and 9 days of storage, whereas unbound free phage under similar conditions followed the expected pathway of desiccation and 100% inactivation⁴.

CONCLUSIONS

Controlled synthesis enables reproducible production of nitrocellulose nanoparticles and metallic nanocomposites. Particle surfaces can be functionalized with biological components (viruses and proteins), and preliminary evidence suggests that bound phages are active after drying and rehydration.

ACKNOWLEDGEMENTS

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Preferred Format: Poster Core@shell nanoparticles for stimuli-responsive drug delivery

Jessica. L. Sanders^{*a}, Daniel J. Bell^a, Maria L. Odyniec^a, Christopher M. Williams^a, A. Damien Walmsley^b, Sarah A. Kuehne^b, Grace Ball^a, Timothy L. Easun^a, Zoe Pikramenou^a

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Abstract. Stimuli-responsive drug delivery is a promising strategy for localised treatment to combat both bacterial infection and cancer. Hydrophobic drugs have poor activity within the body and are particularly challenging to deliver. We present a range of core@shell nanoparticle designs for stimuli-responsive drug release, based on encapsulation of hydrophobic drugs.

INTRODUCTION

Localised drug release strategies offer a unique advantage over traditional treatments, where off-target side effects can be minimised. Drug release triggered by external stimuli is advantageous to combat both antimicrobial resistance¹ and cancer,² with limitations of current therapies due to nontargeted drug release. Temporal and spatial control over drug release can limit off-target effects, and higher drug concentrations at the target site will allow for administered doses to be lowered. Previous work has been focused on mesoporous nanoparticles (mSiO₂) as they have high surface area with high loading capacity, however, they exhibit uncontrolled untargeted drug release. Nonporous silica nanoparticles demonstrate excellent capabilities as drug delivery agents due to their biocompatibility and easy functionalisation.³⁻⁵

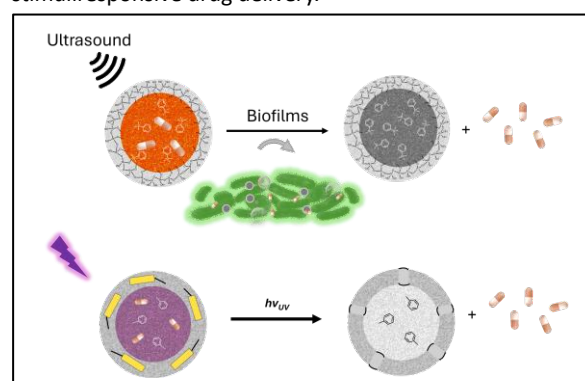
RESULTS & DISCUSSION

Low frequency ultrasound (LFUS) is commonly used in clinic (dermatology, dentistry) and is an attractive versatile stimulus. Silica nanoparticles with encapsulated antibiotics have shown controlled release upon LFUS application, with deeper penetration into biofilms.

For hydrophobic antibiotic rifampicin, a core@shell approach has shown to be more effective than a

'co-condensation' approach.⁶ Recent results in the development of novel photoactive structural frameworks to explore light as a trigger of anti-cancer drug release will be presented.

Figure 1. Core@shell silica nanoparticle designs for stimuli-responsive drug delivery.



CONCLUSIONS

Stimuli-responsive release from non-porous, amorphous silica nanoparticles has been triggered by multiple stimuli to release a range of drug molecules, with an increased efficacy against bacterial biofilms being observed.

ACKNOWLEDGEMENTS

We wish to thank EPSRC grant EP/V028553/1 for support (MO, DB) and EPSRC support for scholarships (JS).

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Preferred Format: Poster Evaluating acoustic wave propagation in hydrogel networks modified via peptide-resinmediated *in situ* gold nanoparticle nucleation

Debsmita Seal^{*a}, Daniel Pastor^b, Finlay J. Douglas^b, Kevin Malikebu^a, Iqra Azeem^a, James Windmill^b, King Hang Aaron Lau^a

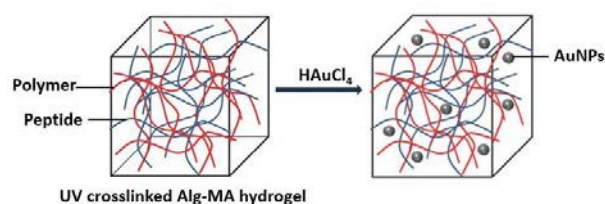
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Abstract.

Developing soft materials to manipulate acoustic waves fundamentally requires tuning mass density to alter acoustic impedance. While introducing high-density nanoscale inclusions is a highly promising approach, conventional physical mixing often causes severe nanoparticle aggregation [1]. Therefore, we utilise a bottom-up chemical toolkit to synthesise gold nanoparticles directly within methacrylate-modified alginate (Alg-MA) networks. Because the abundant hydroxyl groups on the Alg-MA backbone act as mild reducing agents driving competitive background reduction [2], we investigate how distinct embedded peptide-resin domains, specifically a dual reducing and stabilising sequence (YYACAYY) versus a purely stabilising sequence reliant on NaBH₄ for reduction (RMRMKMK) [3, 4], govern *in situ* gold nanoparticle formation. This work focuses on evaluating the impact of the resulting composites on acoustic wave propagation by analysing preliminary ultrasonic transmission data. Such analysis allows us to quantify how localised nanoscale density modifications dictate acoustic attenuation. Initial measurements are conducted by placing hydrogel samples between opposed 1 MHz transducers and quantifying signal attenuation against a reference established using an acoustic couplant.

Figure 1. Schematic illustration of *in situ* gold nanoparticle (AuNP) nucleation within a preformed, UV-crosslinked Alg-MA hydrogel containing embedded peptides. Reproduced from ref [1] with permission.



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Nanoparticle Delivery of Ruthenium Polypyridyl DNA Probes

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ABSTRACT

Nanoparticles (NPs) are versatile materials with promising potential application in the biomedical field.¹ They can be readily functionalised to direct interactions with their environment, which are enhanced by the high surface to volume ratio. Silica nanomaterials in particular have attracted attention due to their biocompatibility, their tuneable properties and their ability to carry a load both internally and externally. This makes them the ideal candidates for cellular imaging in addition to the delivery and controlled release of therapeutic agents. Ruthenium polypyridyl complexes (RuPP) are promising theranostics agents, however, their effectiveness is limited by poor cellular uptake. In this work, silica NPs are considered as delivery platform for these complexes with the aim of controlling their loading and size and exploring how their cellular uptake may differ to the free complex.

INTRODUCTION

RuPP complexes have emerged as promising DNA-binding probes due to their robust photophysical properties which are readily tuned by facile interchangeability of the ligand architecture, enabling control over DNA-binding affinity and selectivity.^{2,3} Their photophysical and photochemical properties make them ideal candidates as both biological trackers and therapeutic agents.^{3,4} Among these is $[\text{Ru}(\text{phen})_2(\text{dppz})]^{2+}$, which is a 'light-switch' complex that has not readily internalised into live cells. However, $[\text{Ru}(\text{phen})_2(\text{dpqa})]^{2+}$ is a derivative complex which incorporates an amide-linked alkyl chain that makes it more lipophilic than the parent complex. However, it has been proven challenging internalising large quantities of these molecules whilst also bypassing endocytic pathway to allow for nuclear localisation without using surfactants that comprise cell integrity. One way to overcome this is to use silica-based scaffolds as a vehicle to load and deliver these complexes into cells.

RESULTS & DISCUSSION

A modified Stöber synthesis involving sequential growth steps was used to prepare ruthenium-encapsulated silica NPs of a size between 35-58 nm (Figure 1).⁵ An orange, opalescent powder (≈ 60 mg) was obtained after centrifugation washing steps. The NPs are readily re-dispersible in water and zeta potential measurements indicate that the NPs are negatively charged & are colloidally stable in aqueous solutions. Furthermore, these NPs absorb in the visible region and exhibit strong photoluminescence under aqueous conditions.

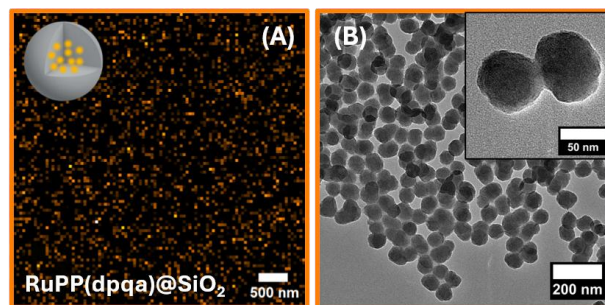


Figure 1 (A) Confocal image of luminescent NPs & (B) TEM image of NPs

CONCLUSIONS

Complex-encapsulated NPs were successfully prepared which exhibited strong luminescence and have shown good colloidal stability under aqueous conditions.

ACKNOWLEDGEMENTS

H.S. acknowledges financial support from the UCD School of Chemistry & Research Ireland (21/FFPP/10126 and 12/RC/2275)

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Preferred Format: Oral Field-Responsive Self-Healing Coatings Based on Magnetic Nanoparticles

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Abstract. The study explores the development of protective coatings based on magnetic nanocomposites with self-healing functionality induced by an applied alternating magnetic field (AMF). It covers the synthesis and characterisation of magnetic nanoparticles (MNPs), the design of responsive coating systems, and testing of their functionality under a high frequency AMF. The concept is based on the ability of MNPs to induce localised heating when exposed to the field, which enables rearrangement of the polymeric coating matrix. The work demonstrates a promising route towards more durable coatings that can extend material lifetime and support sustainability.

INTRODUCTION

Protective coatings play a critical role in extending the service life of engineering structures exposed to aggressive environments. However, conventional coatings often lose their effectiveness once microcracks or mechanical defects appear. To address this limitation, selfhealing protective coatings [1] have attracted significant attention as an advanced strategy for improving durability, reducing maintenance needs, and promoting sustainability.

This study focuses on the development of selfhealing protective coatings based on magnetic nanocomposites. The main objective is to investigate how the integration of magnetic nanoparticles can promote autonomous repair in a polymer-based coating.

RESULTS & DISCUSSION

Magnetite-based MNPs were synthesised via the co-precipitation method, functionalised to improve particle–polymer interactions, and integrated into a commercial thermoplastic

polyurethane matrix, with an MNP loading of 15 wt.%. The coatings were tested on carbon fibre-reinforced epoxy substrates commonly used in the automotive and aerospace industries. The synthesised particles and developed coatings were characterised structurally, morphologically, and magnetically.

Self-healing functionality was investigated by exposing artificially scratched coatings to a highfrequency AMF while monitoring the temperature via a thermal camera. Healing was assessed using a stereo microscope and a 3D optical profilometer. The results demonstrated that MNPs field-induced localised heating enabled rearrangement of the coating matrix and controlled repair of defects within 15 minutes without damaging the substrate, whereas the reference coating remained damaged.

CONCLUSIONS

This study demonstrates that field-responsive magnetic nanocomposite coatings offer a promising strategy for self-healing, extending material lifetime and supporting more sustainable protective systems.

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Preferred Format: Oral

Magnetically Actuated SERS Nanosensors for the Rapid Detection of Contaminants of Emerging Concern in Water

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Abstract. Contaminants of Emerging Concern (CECs) — including pharmaceuticals, endocrinedisrupting chemicals and PFAS — threaten water resources at ng/L concentrations, yet conventional LC-MS monitoring is costly, slow and unsuited to field use. Here we present initial work on a magnetically actuated Surface-Enhanced Raman Spectroscopy (SERS) nanosensor platform for rapid, sensitive CEC detection. Raspberry-like composites assemble gold nanoparticles onto magnetic bead cores; an external field concentrates the nanosensors in situ, overcoming diffusion limits without sample pretreatment. The dense AuNP shell generates abundant electromagnetic hot spots for SERS fingerprinting, with selectivity engineered via macrocycle functionalisation and measurements enabled by a patterned superhydrophobic/hydrophilic quartz chip.

INTRODUCTION

Contaminants of Emerging Concern (CECs) — including pharmaceuticals, endocrine-disrupting chemicals, and PFAS — threaten global water resources at concentrations as low as the ng/L range^{1,2}, consistently exceeding regulatory safety thresholds in European surface waters yet remaining poorly monitored³. Conventional LC-MS methods are costly, slow, require extensive sample preparation, and depend on specialised operators, limiting their use for routine or field monitoring².

RESULTS & DISCUSSION

We present initial work on a magnetically actuated SERS nanosensor platform for rapid CEC detection, built around raspberry-like

composites in which gold nanoparticles (AuNPs) are assembled onto a magnetic bead core⁴. An external magnetic field concentrates the dispersed nanosensors into a small, dense detection volume in situ, overcoming diffusion limitations and boosting analyte capture without drying or sample pretreatment. The dense AuNP shell generates abundant electromagnetic “hot spots” for SERS fingerprinting at ultra-low concentrations⁵. Reproducible, low-volume measurements are enabled by a patterned quartz chip, where hydrophilic zones within a superhydrophobic background confine sample droplets to precise positions for parallel acquisition.

CONCLUSIONS

This raspberry-like AuNP–magnetic bead platform offers a promising route towards field-deployable, reagent-free SERS monitoring of CECs in water. Ongoing work targets macrocycle-based selectivity and validation against LC-MS.

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Preferred Format: Poster

Exploring Prussian Blue Hybrid Nanostructures for Photocatalytic Degradation

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Abstract. There is an ongoing need for photocatalytic methods capable of targeting challenging wastewater pollutants such as those produced by the petroleum industry. Prussian blue (PB) is an attractive material for photocatalysis due to its optical absorption range, mixed $\text{Fe}^{2+}/\text{Fe}^{3+}$ redox centres and charge transfer properties, which provides opportunities to promote the generation of reactive oxygen species. Here, initial exploration of Au@PB core-shell nanoparticles and ZnO/PB nanocomposites is described. Photocatalytic behavior was evaluated using methyl orange and methylene blue as model substrates, before extending the study to anthracene as a more challenging substrate relevant to petroleum wastewater.

INTRODUCTION

Chemical industries produce large amounts of wastewater containing persistent pollutants such as molecular dyes and polycyclic aromatic hydrocarbons. Photocatalytic wastewater treatment offers a sustainable approach for degrading these pollutants. However, singlecomponent photocatalysts such as ZnO are limited by wide band gaps and rapid recombination of photogenerated electron-hole pairs, which reduce its photocatalytic efficiency¹. Instead, nanocomposites offer an opportunity to expand the effective photon absorption range, tune the photonic bandgap and improve charge separation.

Prussian Blue (PB) has been widely explored for applications in sensing, energy storage and catalysis.² However, PB incorporation into nanocomposites for photocatalytic applications has been very limited with only one reported example of ZnO-PB based system, alongside PB/TiO₂ and PBA/Cr₂O₃ nanocomposites for photocatalytic pollutant degradation.³⁻⁵

Here, we report initial results on the synthesis and application of Au@PB core-shell and ZnO/PB nanocomposites. Methyl orange and methylene blue dyes were used as model substrates for comparative assessment before then exploring anthracene as a model for polyaromatic substrates.

RESULTS & DISCUSSION

Two PB-based nanocomposites were prepared using different approaches, Au@PB through a multistep synthesis and ZnO/PB through NP coassembly. Both nanocomposites were characterized using UV-Vis spectroscopy, DLS and zeta potential measurements. Nanoparticle tracking analysis (NTA) was used to estimate the particle concentration of the colloidal samples. Photocatalytic performance was compared under controlled conditions, using the same catalyst and pollutant concentrations for each system. UV and visible irradiation were investigated to determine the influence of the light source, alongside experiments with and without H₂O₂ to assess the effect of an additional oxidant. Photocatalytic degradation was monitored by measuring changes in pollutant absorbance over time, with degradation efficiency calculated relative to the initial absorbance.

CONCLUSIONS

PB was successfully incorporated into Au and ZnObased nanocomposites. Au@PB showed enhanced activity under UV irradiation, while ZnO/PB outperformed individual ZnO and PB nanoparticles.

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