5th Annual Inter CDT Conference 2024

Durham
University

SOFI² CDT
EPSRC Centre for Doctoral Training in Soft Matter for Formulation and Industrial Innovation

THE UNIVERSITY of EDINBURGH

UNIVERSITY OF LEEDS

Materials Advances

Soft Matter

BIOCHEMICAL SOCIETY

NEPA
North East Polymer Association

Participating CDTs

- SOFI^{2} (Host) - Durham University, University of Leeds, University of Edinburgh
- Nanoscience and Nanotechnology - University of Cambridge
- Molecules to Products - University of Leeds
- Formulation Engineering - University of Birmingham
- Topological Design - University of Birmingham
- lifETIME - Aston University, University of Birmingham, University of Glasgow

Introduction

The Inter CDT conference was first held in June 2018 in collaboration with the Formulation Engineering CDT and SOFI CDT. The conference aimed to be an opportunity for PhD and EngD students performing research in similar fields to connect. In 2019 the conference expanded to include the CP3 CDT (University of Leeds) and the CDT in Additive Manufacturing and 3D Printing (University of Nottingham, Loughborough University, Newcastle University, and University of Liverpool). In 2020 and 2021 the conference was not held due to the pandemic. In 2022 the University of Leeds hosted, and participating CDTs included Formulation Engineering, SOFI^{2}, CP3 and Molecules to Products. 2023 saw Formulation Engineering host the event again with more CDTs than ever are participating.

The SOFI^{2} CDT is hosting the conference in 2024 at Durham University, with attendance from the Nanoscience and Nanotechnology, Formulation Engineering, Molecules to Products, Topological Design and LifETIME CDTs. Over the course of the two-day conference a wide range of scientific disciplines including chemistry, physics, engineering, materials science, food science, and biology.

Moreover, it is very exciting that this year’s event will be sponsored by RSC Materials Advances, RSC Soft Matter, Biochemistry Society and the North East Polymer Association.

Program

The talk sesstions shall be taking place in the chemsitry building CG85 and the poster sessions, ice breaker and coffee will be talking place Scarbrough Café directley outside the lecture theatre.

Thursday 29th August

10:00 - 10:30	**Arrival and Coffee**	
10:30 - 12:00	**Introduction and Icebreaker**	
12:00 – 13:00	**Session 1 – Chair: Mallika Rana**	
12:00 – 12:05	**Pablo del Pozo Lorenzale** - Formulation Engineering	S1: Enhancing Perfume Retention in Fabrics
12:05 – 12:10	**Callum Hutchinson** - Molecules to Products	S2: Structure-Stability Relationships of Model Asphaltene Molecules: Implications of Sulfur Heteroatom Functionality
12:10 – 12:30	**James King** - SOFI^2	L1: Dissolution Behaviours of Cellulose and Silk Fibroin in 1-ethyl-3-methylimidazolium Acetate and Dimethyl Sulfoxide And Processing for Hybrid Films
12:30 – 12:35	**Jad Jaafar** - Nanoscience and Nanotechnology	S3: Modelling Defect Dynamics and Reactions in TMDs
12:35 – 12:55	**Will Ogle** - SOFI^2	L2: DCM Alternatives for use in Steglich Esterifications, for Green and Sustainable Liquid Crystal Syntheses
12:55 – 13:00	**Laurence Brazel** - Nanoscience and Nanotechnology	S4: Exploring Li_2O_2 distribution in $Li-O_2$ batteries
13:00 – 14:00	**Lunch**	
14:00 – 15:00	**Session 2 – Chair: William Ogle**	
14:00 – 14:30	**Anjana Doshi**	Invited Speaker
14:30 – 14:35	**Mallika Rana** - Molecules to Products	S5: Sustainable production design of switch dyes for dispersant-free polyester dyeing
14:35 – 14:55	**Reece McCoy** - Nanoscience and Nanotechnology	L3: 3D Bioelectronic Gut Model for Modelling Pathogenic Enteric Virus Infections in vitro

14:55 – 15:00	**Jingwen Lei** - SOFI^2	S6: 3D-Printing Chromatography Media for Viral Purification
15:00 – 15:20	**Break**	
15:20 – 16:00	**Session 3 – Chair: Saabir Petker**	
15:20 – 15:25	**James Austin** - SOFI^2	S7: Vitrimers: Reprocessable polymers with applications in energy storage devices
15:25 – 15:45	**Martin Screen** - SOFI^2	L4: Crystallising Proteolysis Targeting Chimeras
15:45 – 15:50	**Gerda Luht** - Molecules to Products	S8: Asphaltene sub-fractions and their interactions with calcium carbonate
15:50 – 15:55	**Vinothan Vaheesan** - Topological Design	S9: Introduction to Topological Insulators and their Application in Waveguiding structures
15:55 – 16:00	**Megan Holdstock** - SOFI^2	S10: Understanding the Dispersion Behaviour of Plant Protein Particle Fillers in Non-Aqueous Media
16:00 – 17:15	**Poster Session**	
17:15 – 18:30	**Hotel Check-in – Hatfield Collage**	
18:30 – 19:00	**Drinks Reception – Marco Pierre White**	
19:00 – 20:30	**Conference Dinner – Marco Pierre White**	

Friday 30th August

9:00 – 9:30	**Arrival and Coffee**	
9:30 – 10:00	**Poster Session**	
10:00 – 11:15	**Session 4 – Chair: Buddy Visetthernrakul**	
10:00 – 10:05	**Natalie Richards** - SOFI^2	S11: Investigating Bacteria-Driven Vesicle pH-taxis Through Microfluidics
10:05 - 10:10	**Tahlia Palmer** - Topological Design	S12: Phonons and the Physico-Chemical Behaviour of Organic Crystals
10:10 – 10:30	**Tariq Hussein** - Nanoscience and Nanotechnology	L5: Probing Early Time Crystallisation Kinetics and Photophysics of Colloidal Metal Halide Quantum Dots: A Time-Resolved Microfluidic Flow Study
10:30 – 10:35	**Benjamin Devenish** - SOFI^2	S13: From Tip to Ship: Characterisation of New Marine Antifouling Coatings
10:35 – 10:55	**Sean Mitchell** - Topological Design	L6: Using Machine Learning to Identify Knots
10:55 – 11:15	**Sven van Golden** - Topological Design	L7: Fractal Geometry
11:15 – 11:40	**Break**	
11:40 – 13:00	**Session 5 – Chair: Gerda Luht**	
11:40 – 11:45	**Supreeth Sundar** - SOFI^2	S14: Revealing Multiscale Foam Dynamics: Coarsening and Adhesive Forces at Bubble Contacts of Liquid Foams
11:45 – 12:05	**Saabir Petker** - SOFI^2	L8: A Molecular Dynamics Study Towards Barocaloric Polymer Simulations
12:05 – 12:10	**Aqib Asif** **-** SOFI^2	S15: Understanding the mechanisms of self-cleaning surfaces
12:10 – 12:30	**Buddy Visetthernrakul** - Formulation Engineering	L9: Understanding fluidised bed granulation of high surfactant content powders using experimental and modelling approaches
12:30 – 12:50	**Daniel Mathwin** - Molecules to Products	L10: Chemoenzymatic cascade in flow enabled by continuous liquid-liquid separators
12:50 – 12:55	**Ruairi Phelan** - SOFI^2	S16: Extending the Vicsek model to include hydrodynamic interactions

12:55 – 13:00	**Victoria Byelova** - SOFI^2	S17: Many-Blob Modelling: Coarse Graining Proteins for Network Unfolding Behaviour
13:00 - 14:00	**Lunch**	
14:00 – 15:00	**Session 6 – Chair: Reece McCoy**	
14:00 – 14:20	**Daniel Williams** - SOFI^2	L11: Developing Microcapsules for the Delivery of Cytotoxic Molecules
14:20 – 14:40	**Amaziah Alipio** - LifETIME	L12: Sweet and sticky: Increased cell adhesion through click-mediated functionalization of regenerative liver progenitor cells
14:40 – 15:00	**Erin Holdsworth** - Nanoscience and Nanotechnology	L13: Macrocyclic Covalent Encapsulation of Multi-resonant Emitters for Next-Generation Blue Organic Light-Emitting Diodes
15:00 – 15:45	**Closing Remarks and Awards**	

Poster Allocation

P1	**Amaziah Alipio** **-** LifETIME	Sweet and sticky: Increased cell adhesion through click-mediated functionalization of regenerative liver progenitor cells
P2	**Gerda Luht** **-** Molecules to Products	Asphaltene sub-fractions and their interactions with calcium carbonate
P3	**Adrian Pui Ting Ho** **-** Nanoscience and Nanotechnology	NanoPROTAC to guide and monitor protein degradation in chemotherapy-induced senescence
P4	**James Steele** **-** Nanoscience and Nanotechnology	Characterising Structural Evolution in a Sodium-ion Cathode Material (NaNiO$_2$)
P5	**Supreeth Sundar** **-** SOFI^2	Revealing Multiscale Foam Dynamics: Coarsening and Adhesive Forces at Bubble Contacts of Liquid Foams
P6	**Callum Hutchinson** **-** Molecules to Products	Structure-Stability Relationships of Model Asphaltene Molecules: Implications of Sulfur Heteroatom Functionality
P7	**Lizzie Evans** **-** Topological Design	S=1/2 Kagome Magnets in the Two-Dimensional Limit
P8	**Martin Screen** **-** SOFI^2	Crystallising Proteolysis Targeting Chimeras
P9	**James King** **-** SOFI^2	Dissolution Behaviours of Cellulose and Silk Fibroin in 1-ethyl-3-methylimidazolium Acetate and Dimethyl Sulfoxide And Processing for Hybrid Films
P10	**Andrei Paraschiv** - Nanoscience and Nanotechnology	Engineering replicative behaviour in RNA condensates
P11	**Naomi Crabbe** **-** SOFI^2	Small Peptide-analog Hydrogelators: From Synthesis to Application
P12	**Celia Chen** - Nanoscience and Nanotechnology	Stabilising the active FAPbI$_3$ perovskite within a glassy coordination polymer matrix

P13	**Jad Jaafar** - Nanoscience and Nanotechnology	Modelling Defect Dynamics and Reactions in TMDs
P14	**Ella Sapsford** - SOFI²	Tough meets Stretchy: The Role of γ-Cyclodextrin in Polyrotaxane Materials
P15	**Will Ogle** - SOFI²	DCM Alternatives for use in Steglich Esterifications, for Green and Sustainable Liquid Crystal Syntheses
P16	**James Austin** - SOFI²	Thermal analysis and characterisation of RAFT-synthesised PMA of varying molecular weights
P17	**Mallika Rana** - Molecules to Products	Sustainable production design of switch dyes for dispersant-free polyester dyeing
P18	**Erin Holdsworth** - Nanoscience and Nanotechnology	Macrocyclic Covalent Encapsulation of Multi-resonant Emitters for Next-Generation Blue Organic Light-Emitting Diodes
P19	**Jingwen Lei** - SOFI²	Viral Vector Purification with 3D-Printed Chromatography Media
P20	**Toluwalase Agoro** - Nanoscience and Nanotechnology	Characterising hot carrier effects in ultra-thin solar cells
P21	**Benjamin Devenish** - SOFI²	From Tip to Ship: Characterisation of New Marine Antifouling Coatings

Information for Presenters

A range of scientific disciplines are covered in the conference, so please ensure to explain any technical language used.

Short talks will be 5 minutes long. There is no limit on slides, but please ensure your presentation is no longer than 5 minutes. Long talks are 15 minutes long with 5 minutes of questions.

Please load your talks onto the laptop in the break prior to your presentation session to enable us to adhere to the conference schedule

Information for Delegates

Refreshments, lunch and evening meal will all be provided. Dietary requirements provided during registration have been passed onto the venue, however if you have any additional needs, please contact us. The drinks reception on the 24th includes prosecco, non-alcoholic sparkling wine and soft drinks.

WiFi can be accessed throughout Durham Campus using Eduroam.

Addresses

Hatfield Collage: N Bailey, Durham DH1 3RQ
Durham Chemsitry Department: Lower Mount Joy, South Rd, Durham DH1 3LE
Marco Pierre White Resturant: Hotel Indigo, Old Shire Hall, 9 Old Elvet, Durham DH1 3HL

For any further queries please contact Will (mmwo@leeds.ac.uk) or your Inter-CDT Rep.

Book of Abstracts

Enhancing Perfume Retention in Fabrics

del Pozo Lorenzale, Pablo[1*]; Fryer, Peter[1]; Andreu, Patricia[2], Amador, Carlos[2], Zhang, Zhenyu Jason[1]

*Corresponding author: pxd178@student.bham.ac.uk

[1] School of Chemical Engineering, University of Birmingham, Edgbaston, B15 2TT); [2]Procter & Gamble, Newcastle Innovation Centre, Newcastle-upon-Tyne, U.K. NE12 9TS

Keywords: Formulation, Surfactant, Fragrance, Droplets, Deposition.

Scent is one of the most important factors affecting consumer satisfaction in the fast-moving consumer goods industry. However, the inherent volatile nature of perfume raw materials (PRMs) in formulated products makes retention of perfume oils into woven substrates challenging and not fully comprehended. Previous studies show that deposition and penetration of PRM can be related to the Weber ($W_e=\rho D_0 v^2/\sigma$) and Reynold numbers ($R_e=\rho D_0 v/\eta$), both parameters affected by interfacial tension between droplets and substrates. However, these have not been commonly exploited in industry. By using optical tensiometry, we studied the ability of different surfactants to reduce interfacial tension of PRMs at concentrations of interest, determining which had the largest effect. The study of more droplet properties, such as average droplet size was conducted by using fluorescence labelled PRM to create emulsion that were later deposited into fabrics. Through this new methodology, we provide a simple and comprehensive way of predicting droplet deposition onto fabric substrate which we aim to apply into the new generation of detergent products.

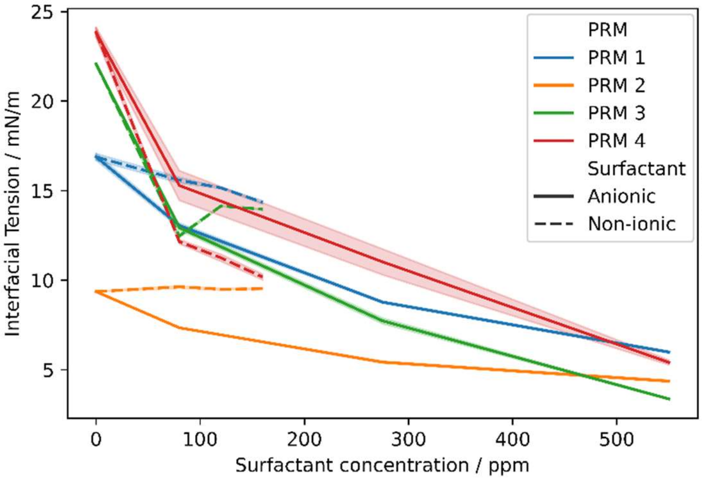


Figure 1. Effect of surfactant concentration on interfacial tension of PRMs and water.

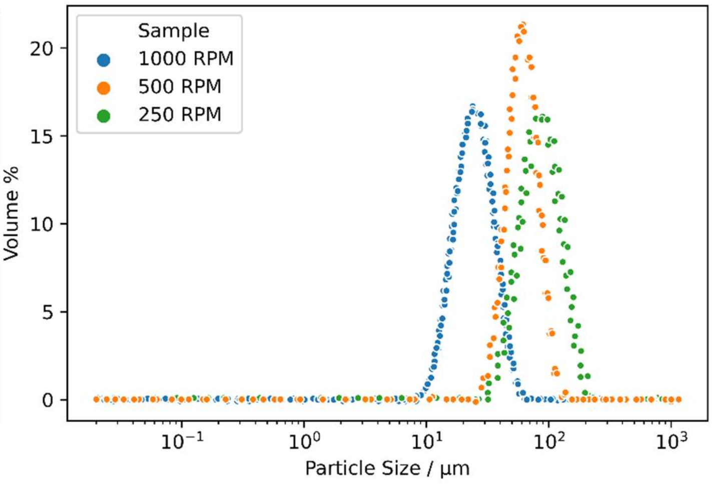


Figure 2. Emulsion droplet size distrubition under 3 different shear conditions.

References:
[1] De Goede, et al. *Phys. Fluids.*, **33**, 033308 (2021).
[2] Argentou, et al. *RSC Adv.*, **12**, 2160 (2022)

Structure-Stability Relationships of Model Asphaltene Compounds: Implications of Sulfur Heteroatom Functionality

Hutchinson, Callum[1*]; Robinson, Tom[2]; Dowding, Peter[2]; Marsden, Steve[3]; Harbottle, David[1]

*Corresponding author: cm16cjh@leeds.ac.uk

[1]School of Chemical and Process Engineering, University of Leeds, UK; [2]Infineum UK Ltd. Oxfordshire, UK; [3]School of Chemistry, University of Leeds, UK

Keywords: Asphaltenes, Structure-stability, Model Compounds

Since 2020, the International Maritime Organisation (IMO) mandated a maximum sulfur content of 0.5% in Heavy Fuel Oil (HFO) to reduce environmental impact [1]. However, this has affected engine performance due to the instability of asphaltenes, which aggregate in aliphatic environments, forming deposits. Asphaltenes can be divided into Interfacially Active Asphaltenes (IAA) and Remaining Asphaltenes (RA) with IAA being particularly problematic due to its enrichment with sulfur and oxygen heteroatoms [2,3]. New insights into asphaltene stability can be gained by synthesizing model compounds to study factors such as molecular weight, functional group chemistry and single/multi-core motifs. A brominated polyaromatic isoquinoline precursor was synthesized to modify for these factors. The model asphaltene compounds, as shown in Figure 1, have been studied using light and neutron scattering techniques to compare aggregation behaviours of motifs possessing a sulfur heteroatom in different oxidation states – sulfidic, sulfoxide and sulfone. The study revealed that oxidized-sulfur compounds aggregate more strongly than sulfidic ones which can provide new direction to develop more effective approaches to mitigate asphaltene stability issues.

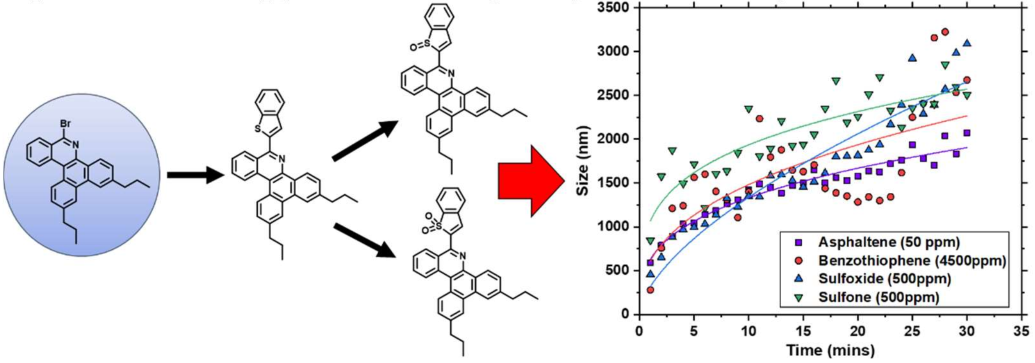


Figure 3: Modification of a 1-bromoisoquinoline substrate into sulfur-functionalised asphaltene-like compounds and its effect on stability

Acknowledgements: I would like to gratefully acknowledge the Engineering and Physical Sciences Research Council (EPSRC – Grant Reference: EP/S022473/1) and Infineum for the funding of this research

References:

[1] International Maritime Organization (IMO), [Online], 2020, Available from: https://www.imo.org/en/MediaCentre/PressBriefings/Pages/34-IMO-2020-sulphur-limit-.aspx
[2] Ballard, D.A., Qiao, P., Cattoz, B., Dowding, P. J., Prevost, S., Alshamsi, M., Charpentier, T., Roberts, K. J., Xu, Z. and Harbottle, D., Energy Fuels, **34(6)**, 6894-6903, (2020)
[3] Ballard, D.A., Chacón-Patiño, M. L., Qiao, P., Roberts, K. J., Rae, R., Dowding, P. J., Xu, Z. and Harbottle, D., Energy Fuels, **34(11)**, 13966-13976, (2020).

Dissolution Behaviours of Cellulose and Silk Fibroin in 1-ethyl-3-methylimidazolium Acetate and Dimethyl Sulfoxide And Processing for Hybrid Films

King, James Andrew[1*]; Hine, Peter J.[1]; Baker Daniel L.[1]; Ries Micheal E.[1]

*Corresponding author: mmjki@leeds.ac.uk

[1]School of Physics and Astronomy, University of Leeds, Leeds LS2 9JT, UK

Keywords: Silk Fibroin, Cellulose, Composite, Ionic Liquid, Biomaterial, Biocomposite, Dissolution, EmimAc, DMSO

Hybrid biopolymer materials could help combat growing issues with plastic pollution, but processing and dissolving these polymers remains a challenge. 1-ethyl-3-methylimidazolium acetate (EmimAc) is a promising eco-friendly solvent but suffers from high viscosity limiting effective dissolution. [1,2] Dimethyl sulfoxide (DMSO) has been proposed as a cosolvent and shown to reduce viscosity and improve dissolution speed with equivalent solvent thermodynamic quality at up to 50 percent weight. [1-3] However, dissolution behaviours for biopolymer blends and in typical processing conditions remain unexplored for this solvent system. Here we report rapid dissolution and maintained solvent thermodynamic quality up to 80 wt % DMSO for microcrystalline cellulose at 100 °C, while unprocessed silk fibers dissolve only at higher EmimAc concentrations. We show that macroscopic dissolution stops before molecular level saturation is achieved by comparison of nuclear magnetic resonance, rheological data, and optical microscopy. Our finding explain discrepancies in solvent composition optimums seen in literature, and helps to improve understanding of biopolymer dissolution. Lastly, blend solutions are used to prepare hybrid films indicating how this work may provide a foundation for effective solvent choice in future biocomposite study.

Acknowledgements: Prof. M. E. Ries, Dr. P. J. Hine, Dr. D. L. Baker

References:
[1] LvY., Wu J., Zhang J., Niu Y., Liu C., He J., Zhang J, *Polymer*, **20**, 53, (2012)
[2] Hawkins J., Liang Y., Ries M., Hine P., *Carbohydrate Polymer Technologies and Applications*, **2**, 100021, (2021)
[3]Tomimatsu Y., Suetsugu H., Yoshimura Y., Shimizu A., *Journal of Molecular Liquids*, **279**, 0167-7322, (2019)

Modelling Defect Dynamics and Reactions in TMDs

Jaafar, Jad[1]; Csányi, Gábor[1]; Hofmann, Stephan[1*]

*Corresponding author: sh315@cam.ac.uk

[1]Engineering Laboratory, University of Cambridge, Trumpington St and JJ Thomson Ave, Cambridge, UK.

Keywords: Oxidation, Defects, Barriers, 2D Materials, WS_2, ML, DFT

Transition metal dichalcogenides (TMDs) are a class of 2D materials that hold potential to transform nanoelectronics. These materials often feature defects that significantly affect their properties. Such defects are pivotal in material oxidation processes, with substitutional oxygen being a notably prevalent defect in TMDs. As exemplified by WS_2, oxidation can either cause unwanted corrosion or be utilized for precise etching and interface creation. Recent studies using operando scanning electron microscopy have revealed that the oxidation of monolayer WS_2 exhibits complex behavior due to various competing mechanisms. This complexity challenges existing kinetic models and calls for a deeper atomistic understanding, prompting the use of machine learning interatomic potential (MLIP) models trained on density functional theory (DFT) data. The introduction of the message passing neural network, MACE, has significantly improved the accuracy of DFT parameterization [1]. Our research involves training a MACE potential for WS_2 to investigate defect dynamics and oxidation processes.

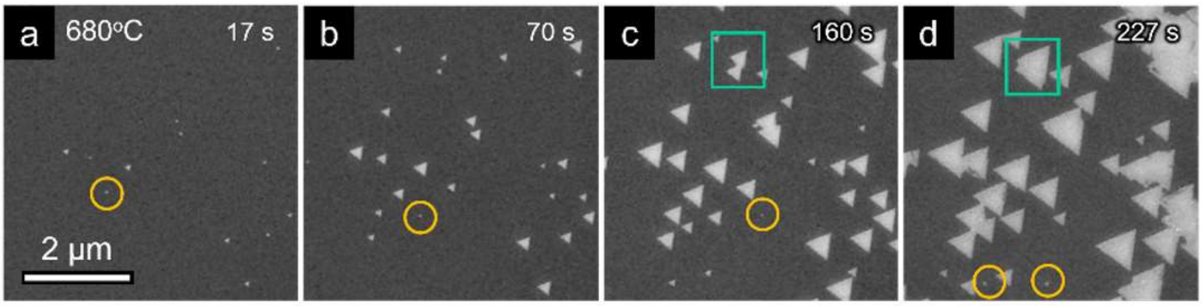


Figure 4: Operando SEM timelapse of WS_2 thermal oxidation

Acknowledgements: SH and JJ acknowledge funding from EPSRC (EP/T001038/1, EP/S022953/1).

References:

[1] Batatia, Ilyes, et al. "A foundation model for atomistic materials chemistry." arXiv preprint arXiv:2401.00096 (2023).

DCM Alternatives for use in Steglich Esterifications, for Green and Sustainable Liquid Crystal Syntheses

Ogle, William[1,2*]; Baker, Daniel L[1]; Ries Michael E[1]; Mandle, Richard J[1,2]

*Corresponding author: mmwo@leeds.ac.uk

[1]School of Physics and Astronomy, University of Leeds, Leeds, UK, LS2 9JT; [2]School of Chemistry, University of Leeds, Leeds, LS2 9JT

Keywords: Organic Synthesis, Sustainability, Green Chemistry, Ferroelectric Nematic

The Montreal Protocol (1989) banned carbon tetrachloride as a solvent due to its ozone depleting properties and was largely replaced by dichloromethane (DCM). [1] Halogenated solvents must now be phased out. DCM is hepatotoxic, neurotoxic, carcinogenic and the cause of at least 85 deaths from 1980 through acute exposure. [2–5] Moreover, it has been shown to damage the ozone layer, [1,5] hence, the US EPA have proposed a ban. DCM needs to be urgently replaced with less hazardous solvents, according to the ACS Green Chemistry Institute Pharmaceutical Roundtable. [5]

We screened twenty green and sustainable solvents to find the most efficacious DCM alternative for the synthesis of ester groups in a typical liquid crystal such as CZP-5-N, [6] with a short list being shown in figure 1. Several factors are considered: yield, safety and health factors, and environmental impact (SHE). For each solvent we performed the synthsis of CZP-5-N on mmol scale using the EDC.HCl / DMAP methodolgy. Reactions were performed four times, to give the indicated yield. The SHE scores were obtained from the CHEM21 and GSK solvent selection guides, [7,8] and normalised to get compariable data. The best performing solvent (dimethyl carbonate) was then used in the synthesis of other common liquid crystal substrates, giving excellent results, even for electron poor phenols. Esters are highly prevalent in the new ferroelectric nematic phase, due to their role in polar conjugation. [9] Therefore, sustainability in this area is crucial for the next generation of liquid crystal materials, such as RM734, DIO and their analogues.

Acknowledgements: The authors thank the SOFI^2 CDT for funding a PhD program for WO; RJM thanks UKRI for award of a Future Leaders Fellowship.

References:

[1] F. P. Byrne, et al., *Sustainable Chemical Processes*, **4**, 7 (2016)
[2] P. M. Schlosser, et al., *Environ Health Perspect*, **123**, 114, (2015)
[3] P. Shah, et al., *Biomass Convers Biorefin*, **12**, 1985, (2022)
[4] EPA Press Office, (2023) (accessed 7 August 2023)
[5] J. Lynch, et al., *Analytical Methods*, **15**, 596, (2023)
[6] H. Schad and M. A. Osman, *J Chem Phys*, **75**, 880, (1981)
[7] D. Prat *et al.*, Green Chemistry, **18**, 288 (2015)
[8] R. K. Henderson *et al.*, Green Chemistry, **13**, 854 (2011)
[9] R. J. Mandle *et al.*, Nat Commun, **12**, 4962 (2021)

Sustainable Production Design of Switch Dyes for Dispersant-free Polyester Dyeing

Rana, Mallika G. S[1,2,3*]; Rayner, Christopher M.[2]; and Blackburn, Richard S.[3]

*Corresponding author: pmmgsr@leeds.ac.uk

[1]School of Chemical and Process Engineering, University of Leeds; [2]School of Chemistry, University of Leeds.
[3]School of Design, University of Leeds.

Keywords: Textiles, Colour Chemistry, Process Chemistry

The process for dyeing polyester has high water usage and produces large volumes of chemical pollution. [1] As polyester is the world's most produced textile, [2] a more sustainable dyeing process will have a large impact on the textile industry's environmental footprint. Therefore, Switch Dyes have been developed to remove the need for polluting dispersants and reduce water and energy use. [3] Switch Dyes achieve this by using carbon dioxide to switch the solubility of dye molecules between the aqueous dyebath and the polyester fibre.

To be able to apply this technology in a real-world scenario and realise the potential benefits, it is imperative to ensure production of these dyes is sustainable and commercially viable. Therefore, even in early development stages, the molecular design of Switch Dyes and their synthesis has been optimised with these considerations to ensure this technology is sustainable by design.

The synthetic route of each dye colour has been designed with minimal steps, starting from widely-available, economical and green chemical reagents. These reaction processes have been designed to follow further green chemistry principles, especially a high energy efficiency and a low process mass intensity. This has led to a significant increase in rate of reaction, and a reduction in the waste from both reaction and purification steps. In addition, reactions have been performed in both batch and continuous reaction systems in preparation for a variety of possible commercial trials.

Acknowledgements: Nathaniel. B. Crompton, Harrison. G. Oates

References:

[1] L. R. Manea, A. P. Bertea and A. Bertea, *IOP Conference Series: Materials Science and Engineering*, **877**, 012062 (2020).
[2] *Preferred Fiber & Materials Market Report 2022*, Textile Exchange, 2022.
[3] N. B. Crompton, H. G. Oates, C. M. Rayner and R. S. Blackburn, *Dye Compounds and Methods Of Using,* UK Pat., P343303GB, 2023.

3D Bioelectronic Gut Model for Modelling Pathogenic Enteric Virus Infections *in vitro*

McCoy, Reece[1]; Hankinson, Jacq[2]; Lulla, Valeria[2]; Owens, M. Róisín[1*]

*Corresponding author: rmo37@cam.ac.uk

[1]Department of Chemical Engineering and Biotechnology, University of Cambridge, CB3 0AS, UK;
[2]Department of Pathology, University of Cambridge, Addenbrookes Hospital, Cambridge UK

Keywords: Bioelectronics, 3D Tissue Models, Enteroviruses, Scaffolds, Tissue Engineering

Human enteric viruses, a diverse array of pathogens recognized for their significant role in global diarrheal disease, pose a considerable public health threat. Their environmental resilience, extensive viral shedding, and transmission via the fecal-oral route underscore the urgency of comprehensive investigation. [1]
To delve into the intricate dynamics of viral interactions, elucidate entry mechanisms, and identify anti-viral interventions that impede host entry, the development of in vitro models which faithfully replicate complexities of the gut becomes imperative. [2]
We have engineered a 3D model of the intestine, intricately hosted on a conducting PEDOT:PSS scaffold.[3,4] This model not only emulates the intestinal epithelial lining more so than conventional 2D models, but also captures the nuances of the lamina propria layer, the connective tissue beneath, which is important due to the crosstalk with the overlying epithelium. Monitoring the barrier's integrity over time is achieved through electrochemical impedance spectroscopy (EIS), offering a profound understanding of the model's response to enteric viruses, including poliovirus-like CVA13.
Our findings reveal the capabilities of our 3D bioelectronic gut models – including sensing virus-induced barrier disruption. We are aiming to demonstrate electrical monitoring of virus-induced cellular extrusion of epithelial cells demonstrating a novel pathway for viral shedding and disease progression along the intestinal tract. [5] This approach holds promise in investigating the contraction of diseases and interrupting transmission pathways, which would be a significant stride towards enhanced public health outcomes.

Acknowledgements: R.M. was funded by an EPSRC Cambridge Nanoscience and Nanotechnology (NanoDTC) Ph.D. studentship (Award EP/S022953/1). This work was supported by the Henry Royce Institute for advanced materials through the Equipment Access Scheme enabling access to the 3D Bioelectronics Suite at Cambridge; Cambridge Royce facilities grant EP/P024947/1 and Sir Henry Royce Institute - recurrent grant EP/R00661X/1.

References:

[1] T.-T. Fong, E. K. Lipp, Microbiology and Molecular Biology Reviews, **69**, 357 (2005)
[2] R. McCoy, S. Oldroyd, W. Yang, K. Wang, D. Hoven, D. Bulmer, M. Zilbauer, R. M. Owens, Advanced Science, 2306727, (2023).
[3] C. M. Moysidou, D. C. van Niekerk, V. Stoeger, C. Pitsalidis, L. A. Draper, A. M. Withers, K. Hughes, R. McCoy, R. Acharya, C. Hill, R. M. Owens, Small Science (2024).
[4] C. Pitsalidis, D. van Niekerk, C.-M. Moysidou, A. J. Boys, A. Withers, R. Vallet, R. M. Owens, Sci Adv, **8**, 4761, (2022)
[5] J. Moshiri, A. R. Craven, S. B. Mixon, M. R. Amieva, K. Kirkegaard, Nat Microbiol, **8**, 629, (2023)

Viral Vector Purification with 3D-Printed Chromatography Media

Lei, Jingwen[1*]; David Cox[2], James Pullen[2], Simone Dimartino[1]

*Corresponding author: J.Lei-12@sms.ed.ac.uk

[1]Institute for Bioengineering, School of Engineering, The University of Edinburgh, Edinburgh UK; [2] FujiFilm Diosynth Biotechnologies, Teesside, UK

Keywords: 3D-Printing, Chromatography, Downstream Processing, Photopolymerization, Viral Vector.

Viral purification is a critical process in the production of vaccines, gene therapies, and viral vectors. However, current industrial chromatographic methods face significant challenges, including low resolution, high pressure drops, and inefficient scalability. [1, 2] Traditional chromatography media, while effective for small molecule purification, are often inadequate for the complex structure and size of viruses. These limitations necessitate innovative approaches to optimize the separation and purification processes.

The a priori design flexibility afforded by 3D printing allows for precise control over the structural and functional properties of the chromatographic medium. In particular, 3D printing facilitates the creation of highly ordered porous structure with uniform flow dispersion and significantly lower pressure drops. [3] The resulting stationary phases are highly befitting for application towards large yet labile viral vectors. [4]

Recent progress in our group has produced novel ink formulations achieving sub-200 μm feature resolution capability. [5] Thereafter, this work continues to optimises the printing technology towards the ultimate resolution of 50 μm, through leveraging the precision and flexibility of Digital Light Processing. This tailored medium is expected to provide selectivity for viral particles through anion-exchange functionalisation while maintaining low pressure drops, thereby enhancing industrial process efficiency and scalability.

Acknowledgements: Jingwen Lei gratefully acknowledges her PhD scholarship from SOFI2-CDT and FujiFilm Diosynth Biotechnology. With many thanks to Mariachiara Conti for her generous help in technical transfer, Andrew Johnston for 3D-printing assistance and Patsy Hazelton for help with FTIR. I would also like to thank Tom Bolland and Vince Verwilligen for their assistance on CAD design and TPMS support.

References:

[1] M. G. Moleirinho, et al., *Expert Opinion on Biological Therapy* **20(5)**, 451–465 (2020).
[2] Z. Jiang and P. A. Dalby, *Trends in Biotechnology*, **41** 10 (2023).
[3] C. Salmean and S. Dimartino, *Chromatographia*, **82** 1 (2019).
[4] M. G. Moleirinho et al., *Separation and Purification Technology*, **254**, (2021).
[5] M. Conti, et al., *Advanced Materials Technologies*, **8** 19 (2023).

Vitrimers: Reprocessable Polymers with Applications in Energy Storage Devices

Austin, J.R[1*]; Warren, N.J [2]; Baker, D.L[1]; Mattsson, J[1*]

*Corresponding author: K.J.L.Mattsson@leeds.ac.uk

[1]School of Physics and Astronomy, University of Leeds, Leeds, LS2 9JT, West Yorkshire, UK; [2]School of Chemical and Process Engineering, University of Leeds, Leeds, LS2 9JT, West Yorkshire, UK

Keywords: Vitrimer, Dynamic Cross-linking, Relaxation Dynamics, Energy Storage

A new class of polymers known as vitrimers has received increasing interest in recent years. Based on associative dynamic exchange reactions, the covalent adaptable networks formed by this type of material display comparable properties to traditional thermoset polymers including thermal and mechanical stability as well as ease of processability [1]. Due to the dynamic nature of these crosslinks, these materials also display an array of additional qualities such as self-healing and increased responsiveness to several external stimuli. It is also due to the replacement of static crosslinks that allow vitrimers to possess a similar aptitude for reprocessing to that of thermoplastics; an improvement on their thermoset counterparts.

Since their inception more than a decade ago, a variety of bond exchange mechanisms and polymer networks have been discovered and studied [2]. However, the fundamental studies in literature to describe and model these types of materials are limited. Additionally, much of current research aims to replace current widely used thermosets for the goal of sustainability as opposed to determining additional potential applications. The development of new applications is critically dependent on understanding the underlying nature and dynamics of these systems. Therefore, an outline to determine the behaviour of vitrimers will be established in the context of a potential application in energy storage and batteries [3]. Prepared by a combination of RAFT polymerisation and polymer functionalisation, vitrimers will be characterised in detail by a myriad of techniques such as Broadband Dielectric Spectroscopy, Dynamic Mechanical analysis, and both Small and Large X-ray Scattering (SAXS/WAXS) in order to further understand the structure and relaxation dynamics of vitrimers and vitrimer-like materials.

Acknowledgements:

The authors acknowledge the financial support from the SOFI^2 CDT and the EPSRC.

References:
[1] W. Denissen, et al., Chem. Sci., **7**, 1, (2016).
[2] B. Krishnakumar, et al., Chemical Engineering Journal, **385**, (2020).
[3] L.Elbinger, et al., Energy Storage Materials, **65**, (2024).

Crystallising Proteolysis Targeting Chimeras

Screen, Martin Andrew[1*]; McCabe, James F.[2]; Askin, Sean[3]; Wilson, Mark R.[1]; Mahon, Clare S.[1]; Steed, Jon W.[1]

*Corresponding author: martin.a.screen@durham.ac.uk

[1]Durham University, Department of Chemistry, South Road, Durham DH1 3LE; [2]AstraZeneca, F1 Gawsworth, Charter Way, Macclesfield SK10 2NA; [3]AstraZeneca, 1 Francis Crick Ave, Cambridge CB2 0AA

Keywords: PROTACs, Crystallization, Supramolecular, Polymorphism

Targeted protein degradation (TPD) is an emerging therapeutic modality with the potential to tackle disease-causing proteins previously deemed "undruggable" with conventional small molecules. In the 20 years since the conception of a proteolysis targeting chimera (PROTAC), a molecule capable of harnessing the ubiquitin-proteasome system to degrade a target protein, TPD has moved from academia to industry and is attracting substantial interest, with more than 10 PROTACs now in clinical trials. [1] However, PROTACs are very poorly water-soluble and face challenges regarding their development into drug products with sufficient bioavailability. Formulation strategies successfully employed for other poorly water-soluble small-molecule pharmaceuticals, such as amorphous solid dispersions, may help to improve their bioavailability by increasing their solubility and/or dissolution rate. [2] Pre-formulation studies are required first to understand the physicochemical properties of PROTACs before any such strategies can be implemented, since there is very little literature in the nascent field of PROTACs formulation.[2] Understanding the role non-covalent interactions have on both crystal packing and aggregation in solution is an important step for implementing various formulation strategies.

We are currently investigating the crystallisability, stabilisation of amorphous solid forms, formation of cocrystalline and coamorphous solids of a cereblon PROTAC and a set of structurally similar compounds. After a thorough crystallization screening process using more than 40 solvents and various methods including the high throughput encapsulated nanodroplet crystallisation (ENaCt) protocol [3] and micro-electron diffraction, [4] a single-crystal structure of this PROTAC has been determined using synchrotron-source X-ray diffraction, and powder X-ray diffraction experiments show that several other crystalline forms can be reproducibly obtained. Coamorphous solids of PROTACs with small molecules appear to have negligible dissolution advantage, but amorphous solid dispersions with polymers may show a solubility enhancement.

References:
[1] A. Mullard, *Nat. Rev. Drug. Discov.*, **20**, 247 – 250 (2021)
[2] F. Postges, et al., *Pharmaceutics*, **15**, 156 (2023)
[3] A. R. Tyler, et al., *Chem*, **6**, 7, 1755-1765 (2020)
[4] X. Mu, et al., *Annu. Rev. Biochem.*, **90**, 431-450 (2021)

Asphaltene Sub-fractions and their Interactions with Calcium Carbonate

Luht, Gerda[1]*; Harbottle, David[1]; Ross, Andrew[1]; Schroeder, Sven L.M.[1]; Robinson, Tom[2]; Dowding, Peter J[2]

Corresponding author: ll16gl@leeds.ac.uk

[1]School of Chemical and Process Engineering, University of Leeds; [2]Infineum UK Ltd.

Keywords: Surfaces, Marine Fuels, Calcium Carbonate, Asphaltenes

The marine sector currently uses heavy fuel oil (HFO) as its primary fuel source and is expected to continue doing so as alternative fuels such as ammonia and hydrogen begin to be introduced in the form of blends with HFO. HFO is rich in asphaltenes, a class of molecules prone to deposition on surfaces inside the engine, causing issues with engine performance and longevity. These issues are thought to be caused by a sub-fraction of asphaltenes that are strongly surface active, with this fraction named interfacially active asphaltenes (IAA). In addition to metal surfaces we held interest in the interaction of asphaltenes with calcium carbonate, a component of existing fuel additives (Fig. 1a) and a material present in crude oil wells, and how this may contribute to deposition mechanisms.

Using an emulsion separation method, the IAA fraction is separated from the remaining asphaltenes (RA) that are solubilised in toluene. The heteroatoms content is higher in IAA due to the higher oxygen content (Fig. 1c), which from FTIR analysis is associated with sulfoxides and other oxygen functional groups. Such differences promote strong adsorption of IAA on surfaces (including $CaCO_3$) (Fig. 1b). Interestingly, subsequent stages of emulsification to generate RA_x and IAA_x continue to show differences in the heteroatoms content, but the functional group chemistry becomes more similar. Such changes in the functional group chemistry and its effect on asphaltenes adsorbing on calcium carbonate is currently being studied. The overall objective is to design additive systems to prevent asphaltene deposition in marine engines.

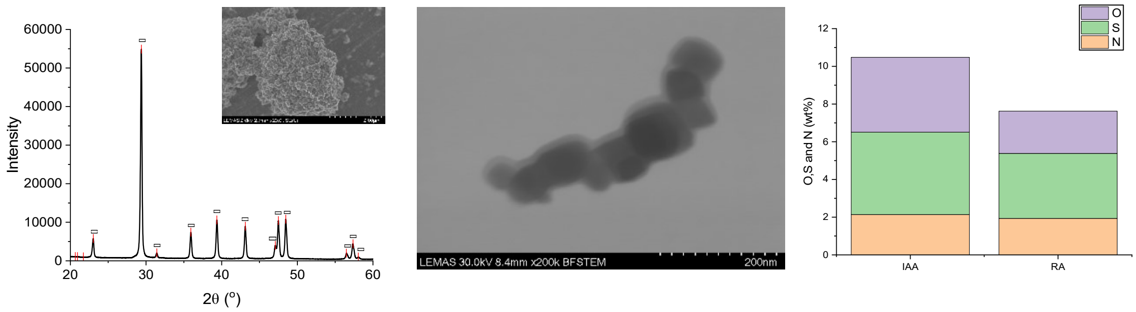


Figure 5: Pure $CaCO_3$ particles (a); asphaltenes adsorbed on $CaCO_3$ particles; and S, N, O elemental analysis of the IAA and RA fractions (c).

Acknowledgements: This research is supported by the Engineering and Physical Sciences Research Council (EPSRC) CDT Molecules to Product grant **EP/S022473/1** and Infineum UK Ltd.

Introduction to Topological Insulators and their Application in Waveguiding Structures

Vaheesan, Vinothan[1,2]*; Navarro-Cía, Miguel[2]; Feresidis, Alexandros[1]

*Corresponding author: vxv762@student.bham.ac.uk

[1]School of Engineering, University of Birmingham, Birmingham, United Kingdom; [2]School of Physics and Astronomy, University of Birmingham, Birmingham, United Kingdom

Keywords: Millimetre Wave, Topology, Photonic Topological Insulator, Meta-surface

The concept of Topological Insulators (TI) has been around since the 1980's with discovery of the Quantum Hall Effect (QHE). The QHE showed that the conductivity is discrete but found that this behaviour could be explained by a special phase (called the Geometric or Berry Phase). The phase was initially proposed by Pancharatnam [1] but was later generalised by Berry for quantum mechanics. [2] The Geometrical Phase is a fundamental concept necessary to describe a TI and its properties. It is a purely geometrical concept but when applied to Condensed Matter systems its topological nature becomes evident i.e. Chern numbers. Under certain conditions, the Chern number can take on non-zero values, in these cases the system is called a Chern Insulator. When a Chern insulator forms a boundary with a material with an unequal Chern number, a fascinating characteristic of Chern TIs occurs on the interface between them. [3] These characteristics are called edge states, they are robust to small changes or impurities and under certain conditions the edge state is “topologically protected”. This introduces the idea of scatter-free propagation.

These applications of topology are not unique to Condensed Matter systems, Photonic systems with band structures and periodic structures are also able to exhibit most of the same topological properties of TI. Applying these concepts of a photonic system, we arrive at Photonic Topological Insulators (PTIs). [4] PTI’s have drawn particular interest in the communications industry for its scatter-free propagation of EM waves. This industry hopes to incorporate PTI’s into the next generation of mobile and satellite communications systems. This seminar will briefly introduce the concepts necessary to understand how Topological Insulators are formed and the fascinating topological properties they inhabit. Concluding with recent research conducted in the practical realization and performance improvements of a metasurface PTI design based on electromagnetic duality.

Acknowledgements: This work was funded by QinetiQ Group plc and the University of Birmingham under the UK EPSRC Grant number EP/S02297X/1.

References:
[1] Pancharatnam, S., *Proceedings of the Indian Academy of Sciences-Section A*, **44***,* 5 (1956).
[2] Berry, M.V., *Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences*, **392***,* 1802 (1984).
[3] Bernevig, B Andrei, *Topological insulators and topological superconductors*, (Princeton University Press, 2013).
[4] Khanikaev, A.B, Shvets, G., *Nature photonics*, **11***,* 12 (2017).

Understanding the Dispersion Behaviour of Plant Protein Particle Fillers in Non-Aqueous Media

Holdstock, Megan[1]*; Murray, Brent S.[1]; Sarkar, Anwesha[1]; Rappolt, Michael[1]; Paximada, Paraskevi[1]; Celigueta Torres[2]; and Powell, Hugh[2].

*Corresponding author: fsmho@leeds.ac.uk

[1]School of Food Science & Nutrition, University of Leeds, Leeds, UK; [2]Nestlé PTC, York, UK.

Controlling the dispersion of solids in non-aqueous media such as oils poses a considerable challenge, particularly when the particle is amphiphilic in nature. This work has set out to develop a better understanding of such materials in the context of a filled fatty matrix: chocolate with added insoluble plant protein particles. In this application, both texture and crystallization properties are crucial in formulating products that meet consumer expectations.

The dispersion behaviour of such plant protein particles in oil was studied using rheological techniques and compared to a model colloidal system; silica nanoparticles with known surface chemistry. Mechanical treatment was used to reduce the inherently large size of protein particles to submicron range, ensuring a desirable mouthfeel. Protein particles formed tightly bound aggregates which were poorly wetted by oil and had minimal effect on the viscosity of the system, whereas low (< 1 vol.%) volume fractions of silica particles increased the viscosity considerably. Small- and wide-angle x-ray scattering were employed to determine the effect of these colloidal particles on the crystallization properties of cocoa butter. The crystal structure of cocoa butter polymorphs were unchanged by the addition of both particle types, indicating that they remain in the fluid phase and do not integrate into the crystal structures. Such particles did, however, exhibit a tendency to enhance crystal growth at sufficiently high volume fractions (> 2.4 vol.%). Oscillatory rheology was also used to probe the temporal evolution of isothermal cocoa butter crystallization and evaluate the effect of particles on fat crystal networks. Comparison of these systems shows that the dispersion behaviour of the two particle types in oil differs, likely due to differences in particle size and surface chemistry. These findings were applied to more complex multi-particle confectionary systems with the aim of creating a material with desirable texture and melting attributes.

Acknowledgements: The Engineering and Physical Sciences Research Council (EPSRC) funded Centre for Doctoral Training in Soft Matter and Functional interfaces (SOFI), Grant Ref. EP/S023631/1as well as Nestlé PTC Confectionary (York, UK).

Phonons and the Physico-Chemical Behaviour of Organic Crystals

Palmer, Tahlia M[1,2*]; Michalchuk, Adam A.L[1]

*Corresponding author: txp390@student.bham.ac.uk

[1]School of Chemistry, University of Birmingham, Edgbaston, Birmingham, B15 2TT; [2]Centre for Doctoral Training in Topological Design, University of Birmingham, Edgbaston, Birmingham, B15 2TT.

Keywords: Thermal Expansion, Phonons, DFT

Temperature plays a key role in energetic materials (EM). However, including temperature in ab initio modelling is challenging. This has hindered our ability to design new EMs in silico. In this work, we attempt to calculate temperature properties using a model EM, FOX-7 (1,1diamino-2,2-dinitroethene), by implementing the quasi-harmonic approximation in ab initio simulations. We show that we can successfully model thermal expansion with good agreement with experimental data obtained from single crystal X-ray diffraction. However, we demonstrate that expansion behaviour can only be captured when thermodynamic entropic corrections are obtained from integrations across the entire Brillouin Zone. Finally, based on our established up-pumping model for impact sensitivity prediction, [1] we show that temperature can therefore be included in the in silico study of EM reactivity.

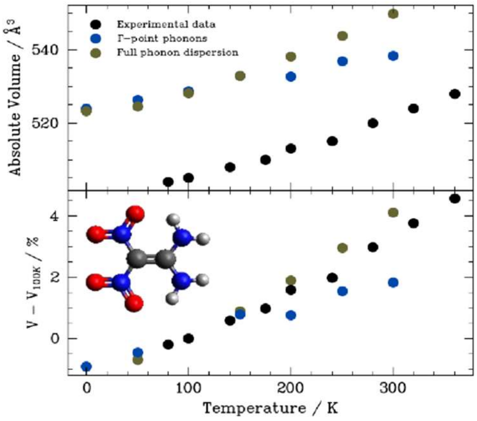


Figure 1: Thermal expansion of FOX-7. The absolute volume vs temperature (top) and the percentage change in volume relative to the volume at 100 K (bottom) for the simulated results using phonons at the Γ (blue) and full integration across the Brillouin Zone (green) compared with experimental data (black).

Acknowledgements: TMP thanks the Centre of Doctoral Training in Topological Design for funding. The computations described in this paper were performed using the University of Birmingham's BlueBEAR HPC service, which provides a High Performance Computing service to the University's research community. See http://www.birmingham.ac.uk/bear for more details.

References:

[1] A. A. L. Michalchuk, J. Hemingway and C. A. Morrison, *J. Chem. Phys.*, **154**, 064105 (2021)

Probing Early Time Crystallisation Kinetics and Photophysics of Colloidal Metal Halide Quantum Dots: A Time-Resolved Microfluidic Flow Study

Tariq Kamal Hussein[1,2]; Bruno Pinho[1]; Samuel Stranks[1,2]; Laura Torrente[1*]

*Corresponding author: lt416@cam.ac.uk

[1]Department of Chemical Engineering and Biotechnology, University of Cambridge, Cambridge, United Kingdom; [2]Cavendish Laboratory, Department of Physics, University of Cambridge, Cambridge, United Kingdom.

Keywords: Perovskites, Quantum Dots, Crystallisation, Kinetics, Photo-physics

Metal halide perovskite quantum dots (QDs) are bright and narrowband emitters that offer outstanding photonic properties based upon the manipulation of their size. [1] Despite this, size control has historically relied upon an empirical methodology (e.g., ligand selection) that lacks true kinetic insight into the transformation rates of precursors and their effect upon final photonic properties. [2] More specifically, the role of coordinating acid-base ligand pairs, such as oleic acid (OA) and trioctylphosphine oxide (TOPO), has been shown to play a pivotal role in modulating size and dispersity; yet to date no studies elucidate the kinetic effects of the acid base equilibrium upon the crystallisation kinetics limiting mechanistic understanding into their. [3,4] To gain rational insight into their crystallisation, a bespoke helical microfluidic platform is developed to time-resolved spectroscopically monitor, in situ, the nucleation and growth of crystallites across three orders of magnitude, from milliseconds to minutes, of synthesis time. By coupling spectroscopic data with 31P and 1H NMR, we find that increased addition of free OA enhances the formation of hydrogen bonded adducts (TOPO-OA) which accelerate consumption of halide salts lending to the formation of highly confined, ~2 nm, monodispersed quasi-spherical QDs at early times (300 ms). Primary growth of crystallites was observed to proceed through a discrete epitaxial, monolayer by monolayer, addition which was found to terminate about a reaction time of 2 seconds yielding quasi-spherical QDs. At late times, 2-5 seconds, crystallites observed facet-limited surface reconstruction evolving into weakly confined (~ 8 nm) cubic nanocrystals. By coupling bulk compositional analysis with time-resolved photoluminescence, we demonstrate secondary growth is consequence of healing of Cs-vacancies resulting in a twofold increase in PLQY (20% to 50%) at much later synthesis times, 10 s. Overall, our study highlights the dual importance of the TOPO:OA equilibrium in crystallising highly uniform bright QDs.

References:

[1] Akkerman, Q et al. *Nat Mater* **17**, (2018).
[2] Pradhan, N. *ACS Physical Chemistry Au* **2**, (2022).
[3] Akkerman, Q. et al. *Science* **377**, (2022).
[4] Almeida, G. et al, J. Am. Chem. Soc. **140**, 44, (2018).

From Tip to Ship: Characterisation of New Marine Antifouling Coatings

Devenish, Benjamin[1*]; Voïtchovsky, Kislon[1]; Heath, Robin[2]

Corresponding author: benjamin.devenish@durham.ac.uk

[1]Ogden Centre For Fundamental Physics, Durham University, Lower Mountjoy, South Road, Durham, DH1 3LE
[2]AkzoNobel, Stoneygate Lane, Felling, Gateshead, NE10 0JY

Keywords: Coatings, Antifouling, Environment, Biophysics, Biofilms, Marine.

Biofouling is a well documented problem on marine structures, such as offshore platforms and large shipping vessels. Fouling of these surfaces can increase costs as well as reduce the operational lifetime of structures, [1] both major issues in marine industries. Current antifouling strategies rely on biocides, such as cuprous oxides, which kill fouling organisms coming in close contact with the coated surfaces during the early stages of biofouling. [2] While effective, this method is known to have detrimental impacts on marine ecology, especially in busy water ways. [3] There is thus a need for new, novel antifouling strategies that do not rely on biocides. One possible solution entails physical methods, whereby the function of the antifouling coating comes from the inability of fouling organisms to attach to the protected surface due to its mechanical and physical properties, such as low surface energies and water contact angles. [4] However, most existing strategies cannot easily be scaled up for routine use in shipping or marine industries. In this research, we investigate a promising new strategy for a polymer-based antifouling coating that combines particular mechanical properties together with nanoscale control of the surface hydrophobicity. This strategy can easily be scaled up, however its specific mode of action and evolution with aging are not yet fully understood. Using Atomic Force Microscopy (AFM) in solution, we characterise differences between candidate coatings, quantifying nanoscale structural and viscoelastic properties that we aim to correlate with the coatings' antifouling performance. These results form a platform for the rational development of functional antifouling strategies to be deployed on a larger scale.

Acknowledgements: This project is partly funded by AkzoNobel Coatings Limited.

References:

[1] Heaf NJ. The Effect Of Marine Growth On The Performance Of Fixed Offshore Platforms In The North Sea. In: Offshore Technology Conference. Houston, Texas: Offshore Technology Conference; (1979)
[2] Michalak I, Chojnacka K. Biocides. In: Encyclopedia of Toxicology. Elsevier; 2014, Pg. 461–3.
[3] Dürr S, Thomason J, editors. Biofouling. 1st ed. Chichester, West Sussex [England]; Ames, Iowa: Wiley-Blackwell; 2010. Pg. 429
[4] Molino PJ, Wetherbee R. The biology of biofouling diatoms and their role in the development of microbial slimes. Biofouling., **365**, 79 (2008

Using Machine Learning to Identify Knots

Mitchell, Sean[1]*; Watkins, Jonathan[1]; Dennis, Mark[1]

Corresponding author: sxm1944@student.bham.ac.uk

[1]School of Physics and Astronomy, University of Birmingham, Edgbaston, Birmingham, B15 2TT, UK

Keywords: Knot Theory, Machine Learning, Topology, Numerical Methods

Knot theory is a field of mathematics which is increasingly being applied to a range of scientific studies such as polymer physics, [1] DNA replication, [2] and colloids. [3] Often these studies wish to establish relationships between a system's properties and the proportion of different knot types appearing within the system. Current numerical methods for finding the type of a given knot are either slow or inaccurate when identifying large knots, which creates incentive to find better algorithms. Other research groups have already made promising progress by showing that machine learning may be able to effectively identify knots. [4] We are hoping to further this progress by combining traditional hand-written approaches with machine learning to achieve higher accuracy when identifying large knots without compromising on speed. Once finished, we will publish the code as a library usable in both Julia and Python.

Figure 6: An example of a distorted knot generated to train the machine learning algorithm. The colour gradient is only to discern which line goes over/under the other and serves no other purpose.

Acknowledgements: Thank you to the CDT in Topological Design and the EPSRC for funding this research.

References:

[1] E. Orlandini, S. G. Whittington, Rev. Mod. Phys., **79**, 611 (2007).
[2] D. Marenduzzo, et al., P. Natl. Acad. Sci. USA, **110**, 20081 (2013).
[3] A. Neophytou, et al., Nat. Phys, **18**, 1248 (2022).
[4] J. Sleiman, et al., Soft Matter, **20**, 71 (2023).

Fractal Geometry

van Golden, Sven Bastiaan[1*]

Corresponding author: sbv373@student.bham.ac.uk

[1]University of Birmingham; EPSRC CDT in Topological Design; Leiden University

Keywords: Fractal Geometry, Iterated Function System, Julia Set

A fractal is a geometric shape that has an infinitely small fine structure; one can zoom in to a fractal at any arbitrarily small scale and still find a rough, detailed structure in it. Fractals arise in many different scientific fields and studying them requires bringing together widely different topics in Mathematics. In this talk I will give a general and non-technical introduction to the mathematical field of Fractal Geometry. Along the way I will show examples of many completely different types of fractals, from the self-similar and self-affine “carpet-like” sets generated by Iterated Function Systems (e.g. the Sierpiński triangle and the Koch snowflake) to Julia sets arising from chaos in complex dynamics (e.g. the Mandelbrot set) and the plane-tiling Rauzy fractals arising from substitutions on symbolic shift spaces.

Revealing Multiscale Foam Dynamics: Coarsening and Adhesive Forces at Bubble Contacts of Liquid Foams

Sundar, Supreeth[1]; Ness, Chris[1]; Royer, John[2]; Lips, Alex[2]; Koutsos, Vasileios[1*]

*Corresponding author: vasileios.koutsos@ed.ac.uk

[1]School of Engineering, The University of Edinburgh [2]School of Physics and Astronomy, The University of Edinburgh

Keywords: Foams, Surfactants, Rheology, Adhesion

This research assessed the effects of aging on the mechanical, rheological, and adhesive properties of liquid foams. Liquid foams are complex materials characterized by a dispersed gas phase within a continuous liquid, stabilized by surfactants. The stability of such foams is influenced by their structural rearrangements over time, particularly through coarsening. Gillette® shaving foam and foam produced by doing a series of ejection/injection cycles of sodium dodecyl sulfate solution through syringe (with stainless steel needle 14G) were used. [1] Rheological studies were done using the Anton-Paar rheometer and adhesive force curves were measured between foam bubbles using an adhesion tensiometer. The results of this study found that (i) at moderate angular frequencies above 5rad/s and below the instrumental limit of 100rad/s the shear moduli agree to the theoretical equations of non-affine bubble motion [2] and the loss modulus follows the scaling law of 0.5. (ii) with aging the elastic modulus shows a clear decreasing trend whereas, the loss modulus initially increases and then decreases which can be interpreted as stages of structural rearrangement and stabilization within the foam. (iii) the adhesive force curves show a repulsive force on contact due to the foam's structure compressing/surface tension effects, and a soft/sublinear response to small displacements. Aged foams showed a smaller elastic scaling factor in the force curves, correlating with the observed decrease in G' over time, which indicates weakening inter-bubble connections. This study provides insights into the dynamic interplay between foam coarsening, viscoelastic properties, and interfacial forces. These findings motivate a deeper understanding of foam dynamics, which is essential for the design and development of more stable and sustainable foam-based products.

Figure 7: Adhesion tensiometry set-up between foam bubbles to capture the bubble-scale dynamics

Acknowledgements: I would like to thank SOFI^2 CDT and EPSRC for the funding and support.

References:

[1] Z Mitrinova, et al., "Surface and foam properties of SLES+CAPB+fatty acid mixtures," *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **438**, 186-198 (2019)
[2] A D Gopal, and D J Durian, "Relaxing in foam," *Physical review letters*, **91**,18 (2003)

A Molecular Dynamics Study Towards Barocaloric Polymer Simulations

Petker, Saabir[1*]; Hobday, Claire L. [1]; Mey, Antonia S. J. S. [1]

[*]Corresponding author: saabir.petker@ed.ac.uk

[1]EaStCHEM School of Chemistry, University of Edinburgh, Edinburgh, UK

Keywords: Barocaloric Effect (BCE), Nitrile Butadiene Rubber (NBR), Glass Transition Temperature (T_g), Adiabatic Temperature Change (ΔT_{ad}).

Current refrigeration processes consume over 20% of the global energy usage and emit high global warming potential gases. [1] This is an unsustainable practice, so new refrigerants must be implemented to avoid further global warming emissions and meet the growing demand. [2] Solid state refrigerants are a long-term solution, with the most promising being materials with a massive pressure-induced caloric effect: barocaloric effect (BCE). [3] The BCE is observed in polymers, and this work focusses on nitrile butadiene rubber (NBR). [4] Using polymers as refrigerants is an exciting avenue towards recycling and reusing otherwise-polluting refuse. [5] There is little experimental work on barocaloric polymers, and fewer computational work, so the exact origins of their large BCEs are unknown. [6] The BCE in polymers is affected by the glass transition temperature (T_g), below which the polymer is in a glass state and above which the polymer is considered a rubber. Below T_g there are low adiabatic temperature changes (ΔT_{ad}), and when pressurising above T_g, ΔT_{ad} increases drastically. We explore the glass transition and its effect on the BCE in NBR using molecular dynamics simulations.

References:

[1] Dupont J. L., *IIF-IIR* (2019)
[2] Van D. Baxter, R Radermacher, *IEA Technology Collaboration Programme* (2020)
[3] J. Garcia-Ben et al., *Chem. Mater.*, **34(7)**, 3323, (2022)
[4] E. O. Usuda et al., *ACS Applied Polymer Materials* **2019** *1* (8), (1991-1997)
[5] A. Gobetti et al., *J Mater Cycles Waste Manag* **26**, 1761–1775 (2024)
[6] L. Cirillo et al., *Thermal Science and Engineering Progress*, **33**, (2022)

Understanding Fluidised Bed Granulation of High Surfactant Content Powders using Experimental and Modelling Approaches

Visetthernrakul, Buddy[1,2*]; Bekto, Hasiba[2]; Ingram, Andrew[1], Simmons Mark[1], Richard Greenwood[1], O'Sullivan Jonathan J.[2]

*Corresponding author: pxv796@student.bham.ac.uk

[1]University of Birmingham, Engineering and Physical Science, Chemical Engineering, Centre for Formulation Engineering, Birmingham, UK; [2]Unilever Research and Development, Port Sunlight Laboratory, Wirral, UK

Keywords: Fluidised Bed Granulation, Surfactant, Response Surface

Powder (anhydrous) formulation of liquid personal cleansing products (shampoo, face/body wash) offers many benefits to both consumers and producers such as greater formula potency, reduced shipping weight and allows for a more sustainable business model. However, high surfactant content is necessary for effective cleansing in powder-based products, but this leads to dustiness and safety concerns due to the small particle size and low density of the surfactant. To address this, the fine particles must be agglomerated with a binder into larger discreet granules in a process called granulation. Granulation is a multifaceted process, and while there is not a single universal model that explains it from first principles, researchers and practitioners often turn to empirical methods. Response surface method has been employed to establish linear and quadratic relationships between the binder particle size, B/S and granulation time to various critical quality attributes.

In situ fluidized bed granulation with a molten binder has been shown to produce highly spherical agglomerates as an alternative to high-shear mixers, however, most granulation literature often uses active pharmaceutical ingredients or standard ballotini (glass) beads [1, 2] which leaves the domain of surfactant granulation unstudied. The investigated variables were binder particle size (45, 187.5, 337.5µm), binder-to-solid ratio (B/S) (22, 26, 30 %w/w), and granulation time (3, 7.5 or 12 min). The experiments were performed in a randomized order according to the Box-Behnken design, giving a total of 15 experiments. Analysis of variance (at the 0.05 level of significance) was performed to determine the significance of each factor. The response variables were the yield, coarse level, fines level, mass median diameter (d50), span (S90-10), poured bulk density (PBD), dynamic flow rate (DFR), spouted bed test (SBT), and solubility (T90) test. Response surface analysis of the data was performed using JMP® statistical analysis software.

Key factors impacting the product quality were binder particle size, B/S, and granulation time. The range of binder particle size and B/S used led to higher yield, but also significant over agglomeration. The binder particle size has linear and quadratic effect on the yield while the B/S only has a linear effect where increasing B/S led to lower yield. The granulation time is the only factor that has a significant effect on the fines level. Overall, most responses were in the desirable range except for the granule size parameters and granule attrition. The study underscores the need for careful control of these parameters for optimal product quality.

References:

[1] H. Zhai, et al., Chemical Engineering Journal. **164(2)**, 275-284 (2010).
[2] I. Aleksić, et al., International Journal of Pharmaceutics. **466(1)**, 21-30 (2014)

Chemoenzymatic Cascades in Continuous Flow Enabled by Continuous Liquid-liquid Separators

Mathwin, Daniel[1,3]; Adam, Anna[4]; Muldowney, Mark[4]; Kapur, Nikil[2]; Blacker, John[3]; and Clayton, Adam[1,3*]

*Corresponding author: a.d.clayton@leeds.ac.uk

[1]School of Chemical and Process Engineering, University of Leeds; [2]School of Mechanical Engineering, University of Leeds; [3]School of Chemistry, University of Leeds.; [4]Sterling Pharma Solutions, Dudley, Northumberland, UK.

Keywords: Synthesis, Continuous Flow, Catalysis

One of the major advantages of flow chemistry is the ability to perform multistep synthesis in a single continuous process, which can enhance efficiency and eliminate solvent intensive purification procedures of intermediates. This may be achieved by telescoping high yielding reactions, minimizing impurities, and implementing continuous separation technology. The combination of chemical catalysis and enzymatic catalysis in continuous flow has potential to realise unique and efficient processes for complex molecules, however, seamless telescoping of these two forms of catalysis is difficult due to their divergent reaction conditions. This project aims to utilise the enzyme Candida antarctica lipase B (CALB) to resolve racemic amines, then further functionalise the enantiopure amine via alkylation using the borrowing hydrogen strategy. Continuous liquid-liquid separators developed at the University of Leeds will be key to isolating the enantiopure amine in-between steps and enable a sustainable route to functionalized chiral amines (Figure 1).

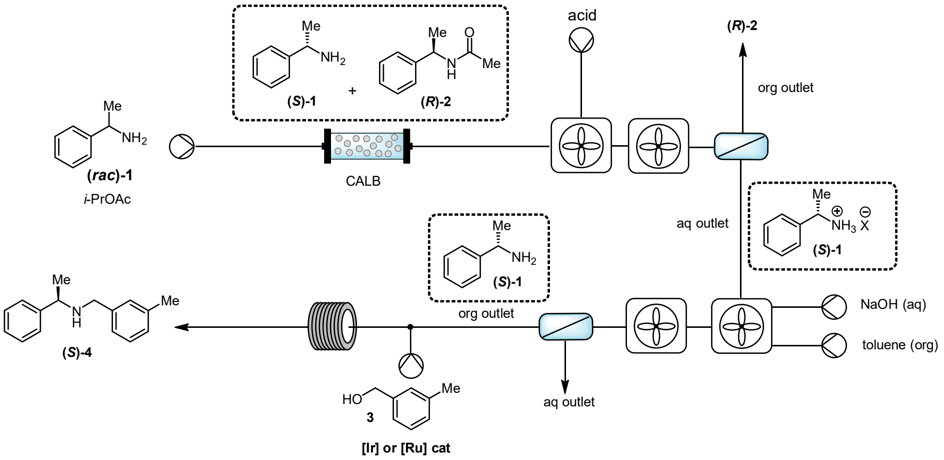


Figure 1. Schematic of the process showing resolution of **1** (***rac***) with CALB followed by isolation of **2** (***S***) using a liquid-liquid separator and then reintroduction into an organic solvent followed by *N*-alkylation using iridium or ruthenium catalysts.

Acknowledgements: Grant Ref. No. EP/S022473/1, Sterling Pharma Solutions

References:

[1] Daglish, J., Blacker, A. J. *et. al. Org. Process Res.Dev.*, **28**, 1979-1989 (2024).

Extending the Vicsek Model to Include Hydrodynamic Interactions

Phelan, Ruairí[1*]; Marenduzzo, Davide[1]; Morozov, Alexander[1]

*Corresponding author: r.p.phelan@ed.ac.uk

[1]School of Physics and Astronomy, University of Edinburgh, Mayfield Road, Edinburgh, EH9 3JZ

Keywords: Active Matter, Collective Motion, Vicsek Model, Bacterial Suspensions

Collective motion is found everywhere in nature, whether that be flocks of birds, schools of fish, or suspensions of swimming bacteria. In recent decades, it has also been extensively studied by scientists as an example of an "active matter" phenomenon that breaks much of the intuition we might carry over from traditional soft matter physics. The most famous mathematical model for this was proposed by Vicsek et al. in 1995, [1] with point particles that move at constant speed and align with their neighbours, while experiencing fluctuations in their orientation. This simple model lends itself to analytical study, while still capturing the behaviour of a whole class of systems.

We build upon an extension to this model [2] to investigate its applicability to microswimmers in a background fluid: first introducing the "run-and-tumble" motion found in bacteria, and then adding in hydrodynamic interactions between particles. By comparing simulations of the "dry" and "wet" models, we can identify if it still falls under the Vicsek universality class, or whether there is a new fundamental change in behaviour.

References:
[1] T. Vicsek, et al., *Phys. Rev. Lett*, **75**, 1226 (1995).
[2] F.D.C. Farrell, et al., *Phys Rev Lett*, **108**, 248101 (2012).
[3] H. Chaté, et al., *Phys Rev E, 77*, 046113 (2008).

Many-blob Modelling: Coarse Graining Proteins for Network Unfolding Behaviour

Byelova, Victoria[1*]

Corresponding author: py19vb@leeds.ac.uk

[1]School of Physics and Astronomy, University of Leeds, Leeds, LS2 9JT, West Yorkshire, UK;

Keywords: Mesoscale, Protein Network, Unfolding, Molecular Modelling

Protein hydrogels are highly biocompatible and stimuli-responsive - their capacity for rational design lends them well to applications such as tissue engineering, drug delivery and wearable medical treatments. [1] Suppressing unfolding of protein domains within a gel leads to generalised behaviour of protein gels at the mesoscale, [2] hence it is possible to use coarse-graining to computationally simulate network formation and behaviour. [3] However, how the process of unfolding affects network formation and behaviour within a protein gel has not yet been addressed, due to the cost of simulation and the difficulty in choosing which properties to keep or discard within the simulation. In my talk, I will outline different network behaviours at play in a protein gel and the challenges of coarse-graining the unfolding process.

Acknowledgements: Dr. David Head, Prof. Lorna Dougan, Dougan research group: Mazin Nazralla, Ahmad Boroumand, Dimitra Katrantzi, Sophie Cawood, Matthew Hughes, Harrison Laurent

References:

[1] A. Zhang, et al., *Chemical Engineering*, **451**, 138494 (2023).
[2] A. Da Silva, et al., *Biomacromolecules*, **18**, 636−646 (2017).
[3] A. Hanson, et al., *Soft Matter*, **15**, 8778 (2019).

Developing Microcapsules for the Delivery of Cytotoxic Molecules

Williams, Daniel[1*]; Lobel, Benjamin[2]; Hughes, Tom[3], Cayre, Olivier[1]

*Corresponding author: py15djw@leeds.ac.uk

[1]School of Chemical and Process Engineering, University of Leeds; [2] Murdoch University, [3]School of Biosciences, York St John's University

Keywords: Drug Delivery, Cancer, Encapsulation

Current clinical doses of chemotherapeutics are substantially greater than required for effective killing of cancer cells. This leads to the drugs having off-site interactions as the drug affects all growing cells, causing severe side effects. Targeted delivery systems, such as encapsulation, aim to minimize unwanted interactions with healthy cells. However, drug leaching and increasing drug payload at tumour sites remain challenges. Reducing off-site interactions and improving targeted delivery are crucial objectives in cancer treatment. Metal-shell capsules are a potential solution for prolonged drug encapsulation and controlled targeted release, due to barrier properties of the crystalline shell preventing diffusion of small molecules from the capsule core to the continuous phase. These capsules can subsequently be fractured remotely using ultrasonic waves, allowing for a non-invasive release mechanism.

Encapsulated Pickering emulsions with controllable diameters (ranging from 100s nm to 10s µm) have been developed using platinum nanoparticles as interfacial stabilisers. The nanoparticles catalyse the reduction of a gold salt for the growth of a localised secondary film around the oil-core. The oil-core permits for the use of drugs with poor aqueous solubility, potentially improving therapeutic outcomes. However, the toxicity and drug loading capacities of the capsules, as well as the efficacy of the ultrasonic release mechanism, have not been fully explored.

Herein, capsules with pharmaceutically appropriate oil-cores which can dissolve concentrations of chemotherapeutics have been developed at biologically pertinent sizes. The toxicity of capsules both unloaded and loaded with varying concentrations of drug dissolved in the oil core have been explored. Finally, the release of the core when exposed to ultrasound has also been investigated.

Sweet and Sticky: Increased Cell Adhesion Through Click-mediated Functionalization of Regenerative Liver Progenitor Cells

Amaziah R. Alipio[1]; Melissa R. Vieira[2]; Tamara Haefeli[3]; Lisa Hoelting[3]; Olivier Frey[3]; Alicia J. El Haj[2*]; Maria C. Arno[1*]

Corresponding author: ara100@student.bham.ac.uk

[1] School of Chemistry, University of Birmingham, Edgbaston, Birmingham, B15 2TT, United Kingdom; [2]Healthcare Technologies Institute, Institute of Translational Medicine, School of Chemical Engineering, University of Birmingham, Birmingham, B15 2TH, United Kingdom; [3]InSphero AG, Wagistrasse 27A, 8952, Schlieren, Switzerland

Keywords: Bio-orthogonal Chemistry, Click-chemistry, Cell Engineering

The burgeoning field of cell therapies is rapidly expanding, offering the promise to tackle complex and unsolved healthcare problems. One prominent example is represented by CAR T-cells, which have been introduced into the clinic for treating a variety of cancers. Promising cell-based candidates have also been explored to promote tissue regeneration, showing high potencies for the treatment of damaged liver. [1] Nevertheless, in the remit of regenerative medicine, cell-therapy efficacies remain suboptimal partly due to the low engraftment of injected cells to the existing surrounding tissue. [2] The selective decoration of cell surfaces with exogenous macromolecules allows for the effective manipulation of cell functions such as adhesion; vital for the improvement of next generation cell therapies. [3,4] In this work, we present a facile approach based on metabolic oligosaccharide engineering [5,6] to enhance the adhesion and engraftment of therapeutic hepatic progenitor cells (HPCs) through specific ligation of exogenous macromolecules to the cell surface without requiring genetic modification. Coated HPCs exhibited significantly increased markers of adhesion and cell spreading, demonstrating preferential interactions with certain extra-cellular matrix proteins. Moreover, they displayed enhanced binding to endothelial cells and 3D liver microtissues. This translatable methodology shows promise for improving therapeutic cell engraftment, offering a potential alternative to liver transplantation in end-stage liver disease.

Acknowledgements: We thank the EPSRC and SFI Centre for Doctoral Training in Engineered Tissues for Discovery, Industry and Medicine (grant number EP/ SO2347X/1) for funding and support.

References:

[1] Lu, W. Y., *et al.*, *Nat Cell Biol.*, **17**, 971-983 (2015)
[2] Forbes, S. J., *et al.*, *J. Hepatol.* **62**, S157-S169 (2020)
[3] Tomás, R. M. F, Gibson, M. I., *ACS Macro Lett.*, **9**, 991-1003 (2020),
[4] Arno, M. C., *Macromol. Rapid Commun.* **41**, 2000302 (2020).
[5] Mahal, L. K., Yarema, K. J. & Bertozzi, C. R. *Science*, **276,** 1125-1128 (1997).
[6] Sletten, E. M. & Bertozzi, C. R. *Acc Chem Res.*, **44,** 666-676 (2011).

Macrocyclic Covalent Encapsulation of Multi-resonant Emitters for Next-Generation Blue Organic Light-Emitting Diodes

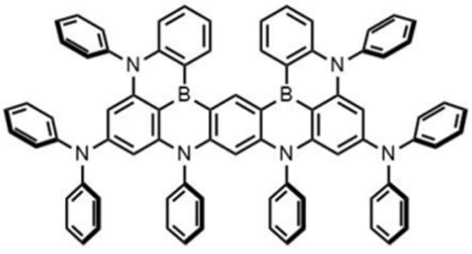
Holdsworth, E. M[1]; Cho, H.-H.[2]; Congrave, D.G.[1]; Bond, A. D.[1]; Riesgo-Gonzalez, V.[1];
Gillett, A. J.[2]; Friend, R. H.[2]; Bronstein, H. A.[1]*

*Corresponding author: hab60@cam.ac.uk

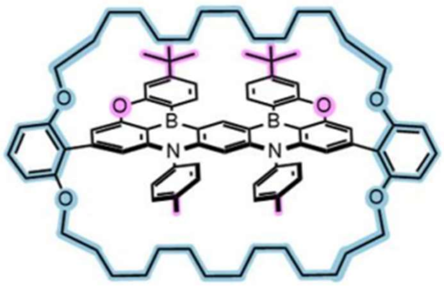
[1]University of Cambridge, Yusuf Hamied Department of Chemistry, Cambridge, United Kingdom; [2]University of Cambridge, Cavendish Laboratory, Cambridge, United Kingdom

Keywords: OLEDs, Optoelectronics, Materials, Synthesis

In the development of next-generation blue organic light-emitting diodes, the MR-TADF emitter ***ν*-DABNA** remains one of the most popular choices for terminal emitters. This interest originates from its assortment of attractive properties, including a high photoluminescence quantum yield, narrowband emission, and the ability to upconvert dark triplet states to bright singlets, namely thermally-activated delayed fluorescence. However, the planar polycyclic structure of this emitter facilitates undesirable aggregate and excimer formation under operational conditions, which significantly limits device performance through a broadening of the electroluminescence spectrum and the establishment of non-radiative energy loss pathways. Furthermore, the commercialisation of these OLEDs is limited by ***ν*–DABNA's** intrinsic sky-blue luminescence which fails to satisfy the current colour standards. Here, these current drawbacks are synthetically addressed by first demonstrating that we can expand upon the current post-borylation chemical space of MR-TADFs to covalently encapsulate a deep-blue ***ν*-DABNA** analogue within a macrocyclic ring, providing the emitters with protection against these detrimental concentration quenching effects. Consequently, fabricating the novel deep-blue emitter into OLED devices based upon the 'hyperfluorescence' strategy boasts an unprecedented external quantum efficiency and Commission Internationale de l'Éclairage coordinate combination of 33% and $y = 0.046$, respectively, ultimately satisfying the BT. 2020 requirement. Overall, we envisage that our 'bottom-up' synthetic strategy represents a promising new paradigm for the development of state-of-the-art OLED materials.



ν-DABNA
Nat. Photon. 2019



EnBOBO
This work

Acknowledgements: This work was supported by the University of Cambridge Harding Distinguished Postgraduate Scholars Program (HDPSP).

Structural Evolution in a Sodium-ion Cathode Material (NaNiO2)

Steele, James M. A[1,2]*; Bocarsly, Joshua, D[3] ; Dutton, Siân. E[2] ; Grey, Clare, P[3]

*Corresponding author: jmas5@cam.ac.uk

[1]Department of Chemistry, University of Cambridge, Cambridge, CB2 1EW, United Kingdom; [2]Cavendish Laboratory, University of Cambridge, Cambridge, CB3 0HE, United Kingdom; [3]Department of Chemistry, University of Houston, Texas, United States of America

Keywords: Battery, Synchrotron, XRD, NPD, Solid-State Nuclear Magnetic Resonance, Crystallography, Energy, Materials, Renewable

Jahn-Teller (JT) distortions, layer glides, and charge ordering during cathode cycling often lead to battery degradation over time. Sodium Nickel Oxide (NaNiO2) serves as a model compound for nickel-rich materials, featuring a Ni3+ JT active ground state, and a plethora of phase transitions during cycling as nickel is oxidised. 1–3 However, the structural evolution of this material and evolution of JT distortion have not been fully understood. Nominally, a series of distorted octahedral (O3x) and prismatic (P3x) phases form throughout charge/discharge. Here, we utilised in/ex situ synchrotron X-ray/Neutron Diffraction (sXRD/NPD) and solid-state nuclear magnetic resonance (ssNMR) to characterise the long- and short-range structures of NaxNiO2 as it charges and discharges. Complementary bulk and local techniques allowed investigation of Na+ vacancy ordering, JT distortion, and structural irreversibilities which occur during charge and discharge. Rietveld refinement of diffraction data has produced the first structural model for the P3A phase, which accounts for TM orbital, and Na vacancy, ordering superstructural reflections. Understanding of the physical processes which occur during cycling of NaNiO2, and the resultant effect on cathode electrochemistry, will inform the design of novel high-performance, nickel-rich NIB cathodes with suitable capacity and lifetime for practical

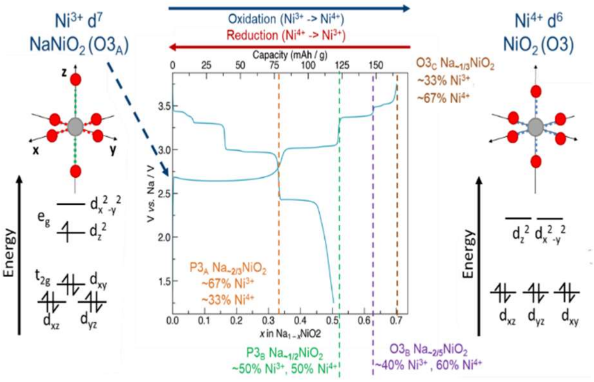


Figure 1: Voltage profile for a $NaNiO_2$ half cell, phase compositions/transitions overlayed. Ideal NiO_6 environments in Ni^{3+} (JT-distorted; d^7 , e_g^1) and Ni^{4+} (non JT-distorted; d^6 , e_g^0).

Acknowledgements: EPSRC Cambridge NanoCDT, EP/L015978/1

References:

[1] P. Vassilaras, X. Ma, X. Li and G. Ceder, J. Electrochem. Soc., **160**, A207 (2012)
[2] M. H. Han, E. Gonzalo, M. Casas-Cabanas and T. Rojo, J. Power Sources, **258**, 266– 271 (2014)
[3] L. Wang, J. Wang, X. Zhang, Y. Ren, P. Zuo, G. Yin and J. Wang, Nano Energy, **34**, 215–223 (2017)

S = 1⁄2 Kagome Magnets in the Two-Dimensional Limit

Evans, E.J[1]; Dolling, T.[1]; Pitcairn, J.[1]; Ivko, S.A.[1]; Manuel, P.[2]; Costantini, G.[1]; Clark, L.[1]*

*Corresponding author: l.m.clark@bham.ac.uk

[1] School of Chemistry, University of Birmingham, Edgbaston, Birmingham, UK; [2] ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, Didcot, UK.

2017 saw the publication of two landmark studies demonstrating the detection of intrinsic ferromagnetism in two-dimensional (2D) layers of CrI_3 and $Cr_2Ge_2Te_6$. [1,2] Since then, there has been growing interest in 2D magnetic materials, whose low dimensionality gives them the potential to host exotic magnetic behaviour and topological states of matter. [3] Magnetic metal-organic nanosheets (MONs) are a class of two-dimensional materials which are highly tuneable [4] and obviate magnetic site disorder; an issue purely inorganic systems often suffer from. [5] In this poster we highlight MOF-bipy ($Cu_3(CO_3)_2(C_{10}H_8N_2)_6 \cdot 2ClO_4$), a layered metal-organic framework (MOF) with S = 1/2 Cu^{2+}-containing kagome layers connected to monodentate ligands in the crystallographic *c*-direction, where these layers are held together by weak intermolecular forces. We determine its crystal structure using single crystal X-ray diffraction and use a combination of magnetometry and neutron powder diffraction (NPD) to elucidate its magnetic structure as ferromagnetic kagome layers which are ferromagnetically correlated to adjacent layers. We demonstrate that the weak intermolecular forces between layers can be overcome using Scotch tape exfoliation, yielding few-layer MONs with lateral dimensions on the order of hundreds of nanometres. These MONs host the potential to be characterised at the 2D limit using surface-sensitive techniques such as X-ray magnetic circular dichroism (XMCD).

References:

[1] B. Huang, G. Clark, E. Navarro-Moratalla, D. R. Klein, R. Cheng, K. L. Seyler, Di. Zhong, E. Schmidgall, M. A. McGuire, D. H. Cobden, W. Yao, D. Xiao, P. Jarillo-Herrero and X. Xu, Nature, **546**, 270–273 (2017)
[2] C. Gong, L. Li, Z. Li, H. Ji, A. Stern, Y. Xia, T. Cao, W. Bao, C. Wang, Y. Wang, Z. Q. Qiu, R. J. Cava, S. G. Louie, J. Xia and X. Zhang, Nature, **546**, 265–269 (2017)
[3] B. Keimer and J. E. Moore, Nat. Phys., **13**, 1045–1055 (2017)
[4] D. J. Ashworth and J. A. Foster, J. Mater. Chem. A, **6**, 16292–16307 (2018)
[5] A. E. Thorarinsdottir and T. D. Harris, Chem. Rev., **120**, 8716–8789 (2020)

Engineering Replicative Behavior into Nucleic-acid-based Membrane-less Synthetic Cells

Paraschiv, Andrei-Alexandru[1]; Di Michele, lorenzo[1,2,3]*

*Corresponding author: ld389@cam.ac.uk

[1]Department of Chemical Engineering and Biotechnology, University of Cambridge, Cambridge, UK, [2]fabriCELL, Imperial College London, London, UK, [3]Department of Chemistry, Imperial College London, London, UK

Keywords: Biomolecular Condensates, Nucleic Acid Nanotechnology, Synthetic Biology

Engineering synthetic cells with the ability to self-replicate represents one of the core objectives of synthetic biology. Despite extensive efforts, no membrane-bound synthetic cell has achieved, to date, integration of all key processes associated with replication, due to difficulties pertaining to in situ sustained ribosomal biogenesis, DNA replication, and controlling membrane division. It is proposed that a synthetic cell system that forgoes the need for a membrane, while still retaining a morphological identity, and spatial and environmental segregation from its environment, could bypass some of the outstanding challenges, and achieve functional and robust replication in a stronger sense than other implementations reported to date. My work is aimed at engineering a membrane-less synthetic cell based on a RNA condensate architecture, capable of replicative behavior that includes growth, genome replication, genome segregation, and division. The work builds on recent advances in programable biomolecular condensates based on co-transcriptional production of RNA nanostructures. [1] Preliminary results probe the landscape of condensate morphologies obtainable in multiphasic RNA condensates.

References:

[1] G. Fabrini, et al., "Co-transcriptional production of programmable RNA condensates and synthetic organelles", *Nature Nanotechnology*, (2024).

Small Peptide-analog Hydrogelators: From Synthesis to Application

Crabbe, Naomi Charlotte[1]; Cobb, Steven Lorimer[1]; Aufderhorst-Roberts, Anders[2*]

*Corresponding author: anders.aufderhorst-roberts@durham.ac.uk

[1]Department of Chemistry, South Road, Durham, DH1 3LE, UK; [2]Department of Physics, South Road, Durham, DH1 3LE, UK.

Keywords: LMWGs, Dipeptides, FMOC-diphenylalanine, Hydrogels, Self-assembly, Biomaterials.

Low molecular weight gelators (LMWGs) that undergo self-assembly have been extensively investigated for numerous biomedical applications owing to their facile synthesis and tunability, low cost, and biocompatibility. [1-5] Among these, Fmoc-FF (9-N-fluorenylmethoxycarbonyl-diphenylalanine) has been the most widely studied model supramolecular hydrogel system, attributed to its rapid self-assembly in response to various stimuli. [6] Much has been revealed about the self-assembly properties of peptides such as Fmoc-FF, but they possess an underlying disadvantage of susceptibility to proteolysis in vivo. [7] This proteolysis results in low bioavailability, and limits their potential use in biomedical applications. N-substituted glycine oligomers, or peptoids, are compounds that mimic peptide behaviour while offering enhanced stability against enzymatic and proteolytic degradation. [7] The fluorenyl and phenyl functionalities in Fmoc-FF contribute significantly to hydrophobic and $\pi-\pi$ interactions, which are crucial for gelation and gel strength, while hydrogen bonding along the peptide backbone plays a less prominent role. [8, 9] Recent findings have shown that similar design principles may also be important in the gelation of N-benzyl glycine substituted Fmoc-FF derivatives. [10] This work aims to demonstrate the straightforward synthesis of Fmoc-FF inspired LMWGs and discuss the design considerations, characterisation methods across multiple lengthscales, and potential applications of these systems.

Acknowledgements: I would like to thank my supervisors, Professor Steven Cobb and Dr Anders Aufderhorst-Roberts, for their support and guidance throughout the beginning of my PhD, and the SOFI^2 CDT for funding this project.

References:

[1] C. Tomasini and N. Castellucci, Chem Soc Rev **42**, 156 (2013)
[2] D. J. Adams, Macromol Biosci., **11**, 160 (2011)
[3] E. K. Johnson, D. J. Adams, and P. J. Cameron, J Mater Chem., **21**, 2024 (2011)
[4] S. Marchesan, Nature, **630**, 308 (2024)
[5] S. Bianco et al., Nature, **631**, 544 (2024)
[6] A. Mahler et al., Advanced Materials **18**, 1365 (2006)
[7] P. L. Nyembe, T. Ntombela, and M. M. Makatini, Pharmaceutics, **15**, (2023)
[8] A. M. Smith et al., Advanced Materials, **20**, 37 (2008)
[9] C. Tang, R. V. Ulijn, and A. Saiani, Langmuir **27**, 14438 (2011)
[10] A. Rajbhandary and B. L. Nilsson, Biopolymers **108**, (2017)

Stabilising the Active Perovskite Phase within a Hybrid Glass Matrix

Chen, Celia[1,2*]; Ye, Chumei[2]; McHugh, Lauren[3]; Dutton, Sian[1]; Bennett, Thomas Douglas[2]

*Corresponding author: cc2147@cam.ac.uk

[1]Maxwell Centre, Cavendish Laboratory, University of Cambridge; [2]Department of Materials Science and Metallurgy, University of Cambridge; [3]Department of Chemistry, University of Liverpool

Keywords: Perovskites, Phase Transformation, Hybrid Glasses, Composites

Lead halide perovskites display exceptional properties for their applications in light-emitting and energy-harvesting. However, their practicality is limited by their phase instability and environmental degradation. [1] Our studies focus on the phase stabilisation of the lead halide perovskite, FAPbI$_3$ (FA = formamidinium), which undergoes a phase transition from the undesired inactive hexagonal δ-phase to the desired functionally active cubic α-phase when heated above 185 °C (Figure 1A). [2] However, heating may not be practical; hence, exploring phase stabilisation at ambient conditions is crucial towards the development of perovskite-based technologies. A promising novel phase stabilisation strategy includes encapsulating the perovskite within a hybrid inorganic-organic glass. (Figure 1B) Previous work from Hou et al. [3] has demonstrated the success of employing a hybrid glass to accomplish phase stabilisation of CsPbI3 due to its excellent interfacial interactions. Furthermore, the vitreous material is neither shape nor size-selective and can conform to the desired shape. Our work demonstrates the success of the hybrid glass encapsulation to stabilise the active phase of FAPbI$_3$ system in the $Zn(H_2PO_4)_2(TzH)_2$ (TzH = 1,2,4-triazole) hybrid coordination polymer.

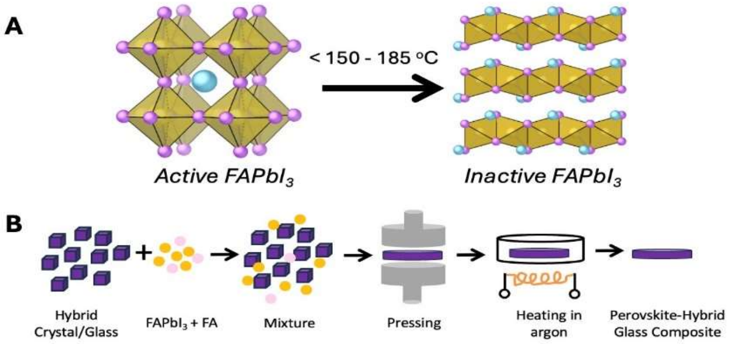


Figure 1: A) Phase transitions of FAPbI3 from the active cubic α-phase to the thermodynamically preferred inactive δ-phase at room temperature and B) Synthesis of FAPbI$_3$-CP composites to achieve the phase stabilisation of FAPbI$_3$

Acknowledgements: EPSRC Cambridge NanoDTC, EP/S022953/1; Leverhulme Trust; Winton Programme for the Physics of Sustainability; and Cambridge Trusts.

References:

[1] S. Masi, et al., ACS Energy Letters, 5, 1974-1985, (2020)
[2] J. Park, et al., Nature, 616, 724-730 (2023)
[3] J. Hou, et al., Science, 374, 621-625 (2021)

Thermal Analysis and Characterisation of RAFT-Synthesised PMA Vitrimer Precursors of Varying Molecular Weights

Austin, J.R[1]; Warren, N.J [2]; [1]Baker, D.L; Mattsson, J[1*]

*Corresponding author: K.J.L.Mattsson@leeds.ac.uk

[1]School of Physics and Astronomy, University of Leeds, Leeds, LS2 9JT, West Yorkshire, UK; [2]School of Chemical and Process Engineering, University of Leeds, Leeds, LS2 9JT, West Yorkshire, UK

Keywords: DSC, TGA, Glassy Relaxations, RAFT Polymerisation, Vitrimer

Thermal analytical techniques have shown themselves to be versatile tools used to analyse the structural properties of a variety of materials and architecture. Differential Scanning Calorimetry relates the heat capacity of a material to its intrinsic dynamics as the material relaxes and undergoes conformational changes. [1] Through this, it is possible to glimpse the behaviour of glassy materials in and around the glass transition or as they begin to flow. Thermogravimetric Analysis is a technique that characterises the weight of a material as a function of temperature or time under prolonged heating. [2] This provides information on the composition and the thermal stability of the material as well as observations of the physical processes that may occur such as sublimation, vaporization, and desorption.

Recent work has utilised Differential Scanning Calorimetry (DSC) and Thermogravimetric analysis (TGA) to determine the thermal stability and characterise the glass transition of a series of RAFT-synthesised poly(methyl acrylate) polymers of differing molecular weights, which are precursors to a set of boronic ester based vitrimers. [3] The variation in their dynamics will be discussed in relation to the changes in these precursors' molecular weights. An understanding of the baseline behaviour and dynamics of these simple systems allows for easier observations of the effects when modifying these systems, such as via copolymerisation or including cross-linking functionality.

Acknowledgements: The authors acknowledge the financial support from the SOFI^2 CDT and the EPSRC.

References:

[1] J. Drzeżdżon, et al., Trends in Analytical Chemistry, **110**, (2019)
[2] N. Saidi, et al., Encyclopedia of Polymer Science and Technology, (John Wiley & Sons Ltd, 2018), pp. 1-29.
[3] L. Huang, et al., Composites Science and Technology, **228**, (2022)

Characterisation of Hot-carrier Effects in Ultra-thin Solar Cells

Agoro, Toluwalase[1*]; Joyce, Hannah[2]; Hirst, Louise[1,3]

*Corresponding author: tmna2@cam.ac.uk

[1]Department of Physics, Cavendish Laboratory, JJ Thomson Avenue, Cambridge, CB3 0HE, UK;
[2]Electrical Engineering Building, 9 JJ Thomson Avenue, Cambridge, CB3 0FA
[3]Department of Materials Science & Metallurgy, University of Cambridge, 27 Charles Babbage Road, Cambridge, CB3 0FS;

Keywords: Hot Carriers, Ultra-thin, III-V Solar Cells

The efficiency of single-junction photovoltaic devices is constrained by the Shockley-Queisser limit to an efficiency of 30% for a bandgap of 1.4 eV. [1] One of the major losses is due to the thermalization of charge carriers, whereby charge carriers relax down to the band edge, via the emission of phonons. A theoretical solar cell called a hot carrier solar cell avoids this loss by delaying the relaxation of charge carriers, thereby keeping charge carriers "hot". [2] Photoluminescence is a powerful tool to probe the energy levels of solar cell absorbers. A Generalised Planck distribution can be fit to the photoluminescence spectra to extract important parameters that relate to charge carrier cooling. III-V thin films have been shown to have delayed carrier cooling thereby keeping charge carriers hot, due to a phonon bottleneck effect. [3]

An 87 nm-thick GaAs solar cell was investigated, and two emission peaks were observed from the photoluminescence. A lower energy peak is thought to be because of the spatially indirect recombination of charge carriers in trap states at the GaAs interfaces. A higher energy peak, observed when the trap states are saturated, is thought to be because of band-to-band transitions. [4] The higher energy emission showed steady-state hot carriers under high-intensity laser illumination. The parameter Q used to quantify carrier thermalization was determined to be 30.46 Wcm^{-2}K^{-1}, with a lower Q signifying slower carrier cooling. Under intense illumination, with higher charge carrier temperatures, a solar cell experiences higher enhancement to the efficiency due to hot carriers. The hot carrier enhancement to the efficiency of the 87nm-thick GaAs solar cell given the determined Q, was calculated to be 0.5% for 100 Suns illumination. Film design optimization to reduce Q and lower the bandgap, as well as high solar concentration, can enable higher hot carrier efficiency enhancement.

Acknowledgements: I would like to thank Dr Eduardo Camarillo Abad and Jiayi Li for fabricating the device studied in this work. I would also like to thank Prof Richard Phillips for the lab space and equipment.

References:

[1] W.Shockley, H.Queisser, In Renewable energy, pages **2** 35–54. Routledge (2018)
[2] R.Ross, A.Nozik, Journal of Applied Physics, **53(5),** 3813–3818, (1982)
[3] Giteau et al, Journal of Applied Physics, **128(19)** (2020)
[4] Hirst et al, Journal of Applied Physics, **117(21)** (2015)