SOFI CDT
EPSRC Centre for Doctoral Training in Soft Matter and Functional Interfaces

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

SOFT MATTERS

August 2021

Soft Matter Showcase 2021 winning poster – Kalila Cook (Cohort 5, Leeds University

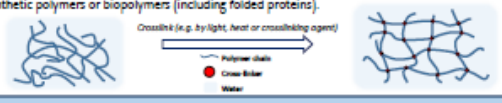
Developing Modelling Tools to Examine Network Formation in Protein Hydrogels

Kalila Cook[1], David Head[3] and Lorna Dougan[1,2]

[1] School of Physics and Astronomy, University of Leeds, [2] Astbury Centre for Structural Molecular Biology, University of Leeds, [3] School of Computing, University of Leeds

1 Hydrogels

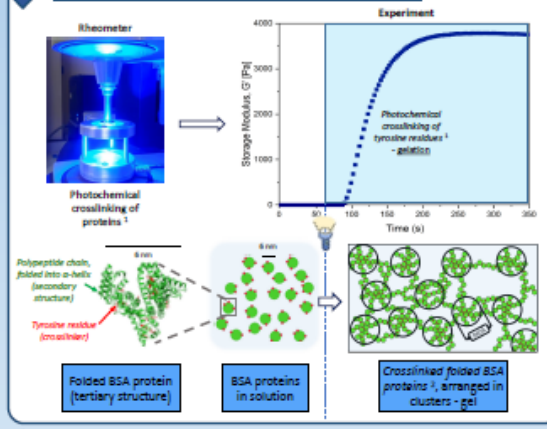
- Hydrogels are hydrophilic polymer networks formed by the crosslinking of polymer chains and subsequent network swelling in water. They can be made from different building blocks, such as synthetic polymers or biopolymers (including folded proteins).



2 Current Aims

- Investigate diffusion-limited cluster aggregation (DLCA) as a crucial mechanism for network formation in protein hydrogels using modelling tools.
- Systematically vary protein density and reaction rate to predict the structure and behaviour of protein hydrogels.

3 Strategy for Hydrogel Formation

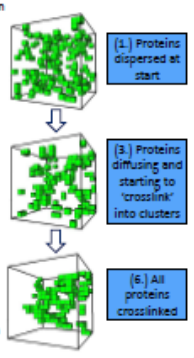


4 Diffusion-limited Cluster Aggregation

- DLCA: proteins, and clusters of proteins, diffuse around and bond irreversibly upon collision

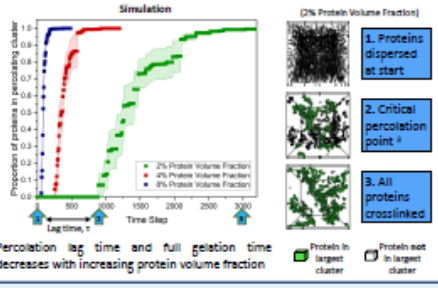
Simulating DLCA:

1. At t_0, a set number of proteins start with random positions in a box of set size
2. Simulation starts: proteins take random walks around box (diffusion)
3. Immediate aggregation (crosslinking) of proteins on contact into small clusters
4. Further diffusion of clusters at rate inversely proportional to their size
5. Further aggregation of clusters into larger clusters
6. At t_{final}, all proteins are crosslinked together: a mega cluster of clusters!



5 Varying Protein Volume Fraction

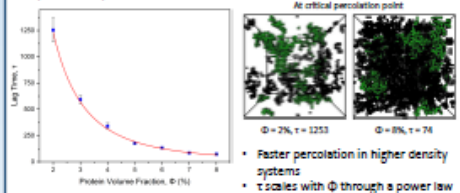
- Percolation: a large cluster of proteins first spans the box



Percolation lag time and full gelation time decreases with increasing protein volume fraction

6 Extracting Lag Time

- Lag time, τ: time elapsed before onset of percolation at the critical percolation point



Power law function:

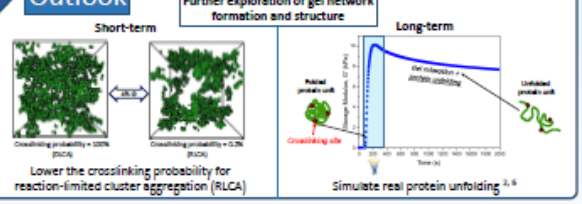
$$y = ax^b$$

Exponent, b = -2.3

- Faster percolation in higher density systems
- τ scales with Φ through a power law function
- Exponent may reveal further details of underlying network formation mechanisms [4]

7 Outlook

Further exploration of gel network formation and structure



Lower the crosslinking probability for reaction-limited cluster aggregation (RLCA)

Simulate real protein unfolding [5,6]

References

[1] Fancy, D.A. and Kodadek, T. (1999). Chemistry for the analysis of protein-protein interactions: rapid and efficient cross-linking triggered by long wavelength light. PNAS, 96(11), p6020.
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[3] Stauffer, D., and Aharony, A. (1994). Introduction to Percolation Theory. Revised 2nd ed., Taylor & Francis.
[4] Ashkenani-Roberts, A. et al. (2020). Reaction Rate Governs the Viscoelasticity and Nanostructure of Protein Hydrogels. Biomacromolecules.
[5] Hughes, M. D. G. et al. (2020). Single Molecule Protein Stabilization Translates to Macromolecular Mechanics of Protein-Nafion-S. ACS Nano.
[6] Khoury, L. R. & Popa, I. (2019). Chemical unfolding of protein domains induces shape change in programmed protein hydrogels. Nature Communications.

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SOFT MATTERS

Note from the Editor

Hi all! What an eventful few months it's been! Hence a slightly longer newsletter than usual, sorry… there are lots of pictures too! The first thing you'll notice about this edition is a new name for the newsletter "Soft Matters"… but more about that on page 3. As always the SOFI/SOFI^2 bunch have been busy with outreach galore, building moves and not to mention the Soft Matter Showcase! This edition has the first contributions from Cohort 7 in the Newsletter so thanks to Jenny Harnett and Luc Dewulf. Also, in case you need a reason to celebrate we have another(!) engagement to celebrate and a competition winner! That's all from me, hope you enjoy this edition and feel free to get in touch with content for the next one!

The Showcase must go on(line)!... Again!

"The same procedure as last year?" "The same procedure as every year!" is what we declared – except this was the Showcase for 80 attendants and not Dinner for One. Just as last year, this year's in-house conference - The CDT Soft Matter Showcase had to be held online for obvious reasons (had we only waited until July 19th …). As opposed to Showcase 2020 however, the (previous) 2-day meeting was shortened to one day to avoid adding to Zoom fatigue. Our approach was "Quality over Quantity".

The Showcase started off with welcoming words from CDT Director Prof Colin Bain with the magnificent interiors of Durham Cathedral as virtual background. Next on air were industrial speakers Dr Jaap den Doelder and Dr Sylvie Vervoort (Dow) live from the Netherlands and Belgium, who presented their real-world experience of plastic recycling in their talk "Pillars of Polymer Circularity". The programme continued with oral student presentations, namely by Adele Perry on liquid crystals, by Lorenzo Metilli on cocoa butter, by Merin Joseph on (theoretical) block copolymers (all from Leeds), and by Jack Williamson on conductive materials (Durham). A highlight of the morning session was the return of SOFI Alumnus Alessandro Gulotta (Cohort 1, formerly Leeds, now a post-doc at the University of Lund) with a presentation of his current research on colloidal approaches to protein mixtures. Good things come in threes, and the morning session closed with three 3-minute flash poster presentations by Kalila Cook on protein hydrogels (Leeds), by Luc Dewulf on the Crover robot (Edinburgh), and by Daniel Williams on nanocapsules (Leeds).

Despite expert advice we had lunch at our desks immersing ourselves in interesting conversations (and our meals) via breakout rooms, before reconvening for the afternoon session. This time we were treated to an account of static fluid columns by Jason Klebes, a presentation of microrheological techniques by Adam O'Connell and by a flawlessly pre-recorded talk on the study of potato cell walls with AFM by Holly Linford (all three Leeds).

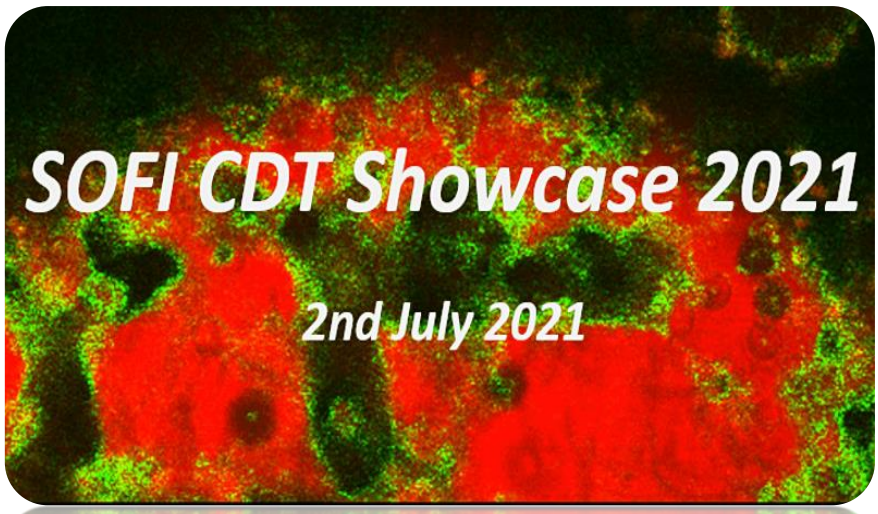
As with any good story, the climax is at the end: Dr David Fairhurst from Nottingham Trent University gave an enthusiastic, entertaining and informative talk on blood spatters and their drying patterns – beautiful but spooky!

The winner of the **3-minute poster presentation** was **Kalila Cook**.

The winners of the **oral presentations** were **Adele Perry** and **Adam O'Connell.**

Congratulations to all winners and a huge thank you to our industrial speakers, external guests, the organising committee and our fellow students!

We are all looking forward to next year's SOFI/SOFI^2 CDT Showcase which will hopefully be in-person or in some hybrid form to enable overseas guests joining virtually. Keep Calm and Stay Soft!



Written by Luc Dewulf, cohort 7

Staff Profile: Professor Megan Povey

Professor Megan Povey is Professor of Food Physics in the School of Food Science and Nutrition at the University of Leeds.

Megan speaking at TUC women's congress on trans rights being human rights.

Megan has developed a range of acoustic techniques for measuring the properties of complex heterogeneous materials such as aero bars, fatty spreads, biscuits and crude oil. She has developed a new method for the tempering of chocolate using high pressure. Currently she is collaborating with Patrick Stowell who is STFC Fellow at Durham and Marcello Galdos at Leeds on acoustic, neutron and electro-magnetic techniques for the characterisation of soils. This is part of the 'Smart Farm' project at the University of Leeds where our unique array of sensors will be deployed on a robot (Developed by Shane Xie's group in engineering at Leeds) housed on the University Farm. Soil condition has a profound impact on plant growth and is part of the GFEI (Global Food and Environment Institute) project on sustainable agriculture. Megan also leads the Food Supply Chain Monitoring theme on the Smart Farm, in collaboration with colleagues at Jiangsu University where we are jointly developing a unique range of very low cost sensors for incorporation in food and food packaging. These sensors are manufactured from common components of foods such as polyphenols (from e.g. beetroot) and are interrogated remotely using very low cost laser diodes. Any monitoring system for food has to be extremely economic and capable of widespread deployment. Her latest project is the development of non-invasive techniques for the measurement of the rheology of materials such as anhydrous milk fat using acoustical techniques.

Megan enjoys gardening in the unique environment of a 60 ° slope on a Pennine Hillside at altitudes between 305 and 290 metre, here the temperatures average 2 °C below that in the valley below, with strong winds and lots of rain. She describes her gardening method as Social Darwinist, the plants either die or survive; depending on natural conditions (weather, soil, other competing plants and animals – the Darwin bit) and on Megan's liking for them (the social and aesthetic bit).Her other hobby is fell running, mostly on the Moor above her farm, where she can imagine running in the footsteps of the Roman runners who ran from Chester to York along the nearby Roman Road, parts of which are still visible. You can learn more about Megan and her work at https://www.insidescience.org/news/pioneering-food-physicist-embraces-new-public-identity.

Competition winner!

In the last edition of this newsletter, we tasked all SOFI/SOFI^2 students and staff to come up with a new name for the newsletter to replace the rather uncreative previous: "SOFI/SOFI^2 Newsletter". Over here at newsletter HQ we expected the entries to come pouring through in their hundreds… alas most of you were far too busy doing real soft matter and we only actually had two entries. BUT, the two entries we did have were excellent! It was a choice between:

- **"SOFI^{-1} Newsletter"** (An intuitive suggestion from the previous name SOFI/SOFI^2 = SOFI^{-1})
- **"Soft Matters"** (A clever play on words!)

In the end, we couldn't decide on a winner so had to take the decision to the management board who voted on their favourite. "Soft Matters" won the vote, so congratulations to the winner who is feeling shy and wishes to remain anonymous!

SOFT MATTERS

Supplementary competition

If anyone out there is a Wizz on photoshop… a new logo to really jazz up these newsletters would be great! Again, no prize, just clout and a sense of achievement!

Outreach: In2Science

In2scienceUK, founded in 2010, promotes social mobility and diversity in science, technology, engineering and maths (STEM). In particular they focus on empowering young people from disadvantaged, low socio-economic backgrounds. Through workshops, online mentoring and placement days, In2scienceUK aims to provide Year 12 students from underrepresented backgrounds with the opportunity to explore a career in STEM, and give them the confidence to pursue a STEM subject at university. In2scienceUK also has a sister organisation called In2research, which is designed to help undergraduate students explore whether a PhD is right for them.

In2scienceUK is partnering with the STEM outreach team at the University of Leeds, hosting a series of 43 online workshops this summer for Year 12 students. One of these workshops is going to feature several of our very own SOFI students!

The workshop in question is titled, 'Opening doors in the Physical Sciences', and will be about the huge variety of different pathways there are to become a research scientist, even when working under the same 'research umbrella' of soft matter. During secondary school, in Year 12 in particular, many young people panic about the big choices they are going to be making, such as whether they want to go to university, and if so, which and to study what! This workshop aims to show the students the interdisciplinary nature that a lot of research in science entails, and how an undergraduate degree in STEM can be a springboard for a whole host of different options and opportunities.

Within the 45 minute workshop, Daniel, Alex, Lorenzo and Holly will be sharing (via video) their journeys from GCSEs (or equivalent) at school to their research today in their PhDs. Students will get a clear picture of the web of interconnected research topics, and see the plethora of experience and types of people within the field of soft matter. I want to say a BIG THANK YOU to Daniel, Alex, Lorenzo and Holly for contributing. Hopefully the workshop will have a lasting, positive impact on the Year 12 students that experience it, and will encourage them to pursue a career in STEM.

You can become a mentor for In2scienceUK in 2022 by registering your interest through the following webpage: https://in2scienceuk.org/volunteers/host-apply/.

Written by Charlotte Pugsley, Cohort 5

Student Profile: Jennifer Harnett

Hi! I'm Jenny from Cohort 7. I'm part of Davide Michieletto's lab group based in Edinburgh and I'm also working with Tilibit Nanosystems - who design DNA origami for academic and industrial applications. My project looks to investigate the rheological properties of DNA origami.

Currently I'm working in Durham with Kislon Voitchovsky, training to use an atomic force microscope to characterise the structure of the origami I have created. Next, I will use microrheology to investigate how different DNA topologies affect rheology, and if any topology-driven collective behaviours arise.

Despite the challenges of starting a PhD during a pandemic, I have really enjoyed being part of the SOFI^2 CDT and starting my project in Edinburgh. I look forward to the future and delving deeper into the world of nano and material science.

Jenny and some of her DNA 'origami'

Alumni Profile: Jon Millican

I joined SOFI CDT in the first cohort in 2014, after doing a degree in Chemistry at York. I enjoyed the cooperative aspect of the SOFI training programme; the most challenging, but also valuable, aspect was communication between students with very different academic backgrounds. This also allowed us to build up a strong network, which grew throughout the program.

My research was carried out at Durham in the group of Prof. Lian Hutchings, and focused on the synthesis of biomimetic functional polymer coatings, inspired by the super-stickiness of mussels. The research was carried out with Epigem, a local SME. One of the most rewarding parts of my PhD was a 10-week international placement at the Leibniz Institute for Polymer Research in Dresden, Germany, which not only provided valuable data for my thesis but also resulted in a recently-published joint paper entitled "Synthesis and characterisation of a mussel-inspired hydrogel film coating for biosensors" - European Polymer Journal 153 (2021) 110503.

After graduation, I have since moved (back) to Germany and am currently working as a Postdoc at the University of Bayreuth, synthesising biodegradable polymers. Our most recent publication was "Plastic Pollution: A Material Problem?" (Macromolecules 2021, 54(10), 4455–4469) which summarises the current issues concerning polymer recycling. It highlights some promising research taking place in the academic community to tackle the plastic pollution problem and the collective responsibility we all face to work towards a circular economy – a topic close to the heart of SOFI/SOFI^2 CDT.

A message from Lian:
…Overseas research opportunity!...

A note from the CDT Manager (and Jon's supervisor) to all CDT students. Overseas research placements for up to 3 months are an option for ALL SOFI/SOFI^2 CDT students. These opportunities are not only of value in enabling you to access expertise and facilities which may not be readily available within the CDT, but are a great personal opportunity to experience life in a different country/culture. Now that travel restrictions are starting to ease, discuss with your supervisor whether there might be a suitable opportunity for you. If you have any general questions about this, please contact the CDT manager (l.r.hutchings@durham.ac.uk).

A(nother) SOFI love story

Clearly the SOFI/SOFI^2 recruitment team moonlight as Cupid's messengers as we have another Soft Matter engagement to announce! A massive congratulations to Will Foster and Vanessa Woodhouse of Cohort 2 who both studied for their PhDs at Durham.

Will Foster was supervised jointly by Halim Kusumaatmaja and Kislon Voitchovsky in the Dept of Physics at Durham and the title of his thesis was "Molecular organisation of water and alcohols at solid-liquid interfaces".

Vanessa was supervised jointly by Beth Bromley (Dept of Physics) and Mark Wilson (Dept of Chemistry) at Durham and her thesis title was "Structure and activity of anti-microbial peptides".

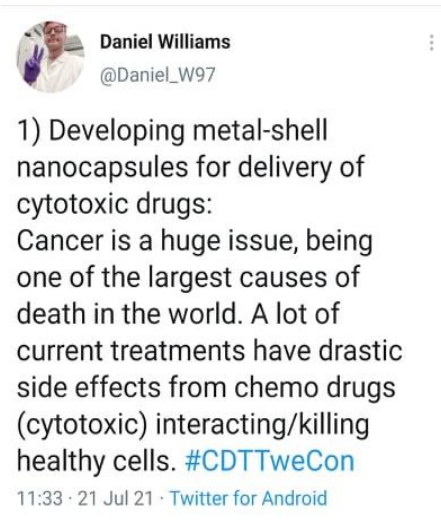
All the best wishes from all of us and we wish you a life of happiness!

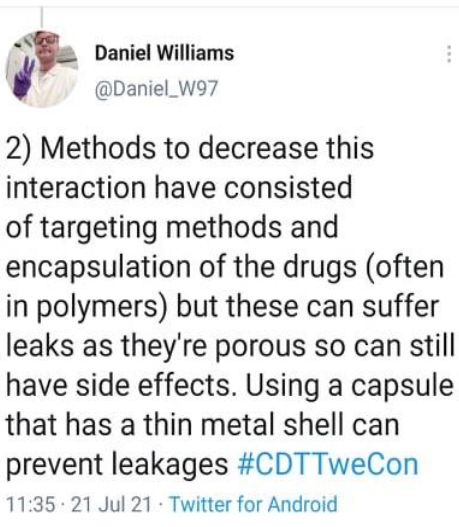
A fond farewell to Prof Rosalind Allen!

We'd like to wish a fond farewell, thanks and best wishes from all the staff and students of SOFI/SOFI^2 to Edinburgh CDT co-director Prof Rosalind Allen, who is leaving University of Edinburgh to take a new position at the University of Jena in Germany! Best of luck in your new position!

Tweet your thesis - SOFI^2 success!

Tweet your thesis: A Leeds based CDT competition ran by the CDTTERM-iMBE in which the entrants had to sum up a bit of their research or project in 3 tweets. The tweets were judged on how they communicated the research, how easy the tweets were to understand, and whether or not it left the audience wanting to know more. There were multiple entries from various CDTs in Leeds with 4 SOFI/SOFI^2 students entering. I managed to win the popular vote with my three tweets summing up metal shell nanocapsules for the delivery of cytotoxic drugs, which can be seen below! A huge congrats to all who took part and let's look forward to the next one!

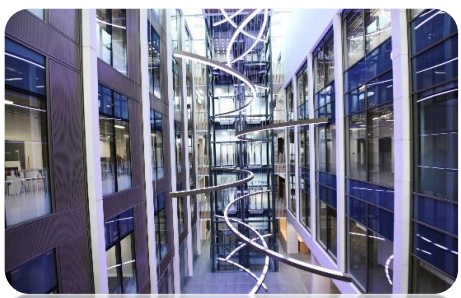




Written by Daniel Williams, Cohort 6

Leeds: Bragging rights

In May 2021, the Physics department at Leeds University began a migration into the brand new Sir William Henry Bragg building! Work began in Spring 2017, with the next four years seeing the construction of state-of the-art laboratories and specialised teaching spaces to enable cutting edge research. Now that the building is complete, work is ongoing hooking up lab equipment and setting up kit across the research groups. Some experiments have also begun, with the Soft Matter department having now opened most of their labs for research and the other departments not far behind. Knowledge of the building move has been looming for as long as any of us can remember, we've seen so many pictures of labs being put together and walked past the building site countless times. Now that's it's finally happening we're all so excited to get started in our new home! Although I think plenty of us will say a sad goodbye to our old home in the EC stoner building and on the Research Deck, even if we won't miss the broken heating system. The experimental officers across the research groups: Dan, Ben and Mannan have had the incredibly tough job of coordinating this effort, and we're all forever grateful to them for their hard work in making this happen.



Written by Adele Parry, Cohort 5

Be Curious: SAW stitching

Written by Kalila Cook, Cohort 5

This year has seen the University of Leeds' annual research open event, 'Be Curious', go online! The 10-day festival in July had a vast programme for children and adults including the 'SAWstitch maker kits' event put together by SOFI/SOFI^2 academics Professor Lorna Dougan and Paul Beales, Kalila Cook (Cohort 5) and Christa Brown.

During this event, free kits could be ordered with all the materials required to embroider your very own self-avoiding walk (SAW) before sharing the result on social media using #SAWstitch. A SAW is a sequence of moves on a grid that does not visit the same point more than once. The purpose of this project was to inspire innovation and discovery by getting people to think about how paths are created and what connections are made along the way. In the wider context, SAWs are used to study how networks form, including social, biological and computational networks and have provided inspiration to artists and designers, so this is a surprisingly wide-reaching topic! To find out more on the science related to SAWs, the relevant work in the Dougan group and how you can have a go at your own SAW-stitching, check out this website!

SAWstitch is a collaborative project and benefited from many enjoyable conversations with the Leeds Physics Craft Gathering group. Our interest in SAWstitch stems from our research on network formation of protein hydrogels. We use biomolecules called proteins as our 'thread' and create networks by making them connect through sticky points on their surface, through photo-activated chemical cross-linking. This results in the creation of a network with a defined shape and material properties.

You can read more about our research here and in this Science highlight here.

We acknowledge funding from the Engineering and Physical Sciences Research Council (EPSRC), Royal Academy Engineering (RAE) and Economic and Social Research Council (ESRC).

Cohort 8(!?)

At the end of this month we welcome another cohort to the SOFI/SOFI^2 gang (I still feel like a newbie being in Cohort 6!). Next edition we'll hopefully have some news about how they've been getting on during their training programme in Durham!

Keep up with all the SOFI/SOFI^2 news online! Find us at www.softcdt.ac.uk

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Feedback and submissions for future issues welcome!
Please contact Alex Gresty at py15allg@leeds.ac.uk