chem@cam

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New term, new scholars, new group leaders

UNIVERSITY OF CAMBRIDGE | Yusuf Hamied Department of Chemistry

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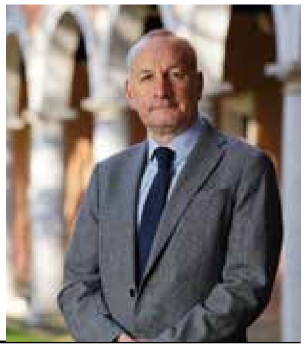

Welcome to the Winter 2023 issue of Chem@Cam

In October we welcomed to the Department around 80 new postgraduate students from around the world. All have amazing records of achievement, and it is a real privilege that so many outstanding graduates choose to start their research careers with us.

This yearly influx of talented and ambitious research students truly is the lifeblood of the Department. In this issue we focus on their achievements, especially those who have been awarded Yusuf Hamied, Gates or Finlay Scholarships. You can also read about the summer projects, generously funded by alumni, undertaken by some of our final-year undergraduates.

In what I think is something of a record we welcome no fewer than three new Assistant Professors to the Department – Pawel Dydio, Ruth Webster, and Julian Willis – as well as two independent early-career fellows, Svetlana Menkin and Mateo Sanchez. In this issue you can read about their research, their plans for the future and what brought them to Cambridge. We expect to hire two more Assistant Professors in the current year, further contributing to a strong sense of renewal.

Our Department could not function without the dedicated and excellent work of the support staff, and in this issue we have the first of a series of articles focusing on their work and the key role they play. The first to be featured is our Head of Housekeeping, Eve Lechowska.

As ever my colleagues are busy with an amazing range of activities, from the Collepardo Group's study visit to Woods Hole, to the continuing success of spinout companies. You can read about these and, of course, other exciting research going on in this issue.

For those who like such things, we offer another of Dr Mary Wood's ever-popular crosswords for you to test yourself against. There is also a reader survey, to which we would appreciate your response by email or even the now old-fashioned postal service.

With all best wishes

James Keeler
Head of Department

Cover photo depicts postdoctoral researcher Sona Krajcovicova

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Chem@Cam is published twice a year, and is sent free to chemistry alumni, postdoctoral researchers, retired staff and friends of the department.

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Meet our Hamied scholars

In 2021, Dr Yusuf Hamied (Christ's 1954) gave a transformational leadership gift to rename the department. This gift included support for a distinguished programme of Hamied scholars at postgraduate level. The first two scholars, who are now in their third year, discuss their progress.

Daniel Warnes (Downing)

Giorio and Vignolini groups

Daniel is exploring the use of cellulose nanocrystals in the atmosphere to counteract global warming.

Geo-engineering is a relatively new field that focuses on manipulating environmental processes to reduce global warming. This includes research into 'solar radiation management,' where clouds are seeded with particles in the troposphere or aerosols injected into the stratosphere, to increase solar radiation reflection and cool the atmosphere.

Daniel, who has a background in Chemical Engineering, was attracted to this project for many different reasons. He says: "This project is massively up my street, combining fighting climate change, engineering and novel materials."

Daniel is working with aerosols derived from cellulose, one of the most abundant materials on the planet, which is also completely biodegradable and safe for humans. "Something that was important to me when I took this on was to not only focus on whether it would work, but to also look at the secondary effects on the flora, fauna, the atmosphere and ultimately humans," he says.

"Some geo-engineering is concerned with putting pretty horrible particles like titanium dioxide into the atmosphere. Chemicals do wash out of the atmosphere, so it's important to look at where they might end up and what happens if they're inhaled by humans."

The combination of supervisors for this project is ideal. "Dr Giorio's group researches air quality and its effect on public health, whilst Prof Vignolini's group looks at photonic and biodegradable materials inspired by nature," says Daniel. An extra bonus is that both supervisors originate from Italy and always have great food and coffee on offer. "It's really welcome," he smiles.

Daniel is grateful that the Hamied scholarship made his research possible. "There is zero chance I would have been able to pursue this area of research without the scholarship."

Daniel says he has made good progress. "Firstly, I've found that it's completely possible to control the aerosolisation of cellulose. The second part that I'm looking at now is whether we can improve light scattering away from earth. The third part will be the connotations for the environment and humans."

However, Daniel emphasises: "I strongly believe that behavioural change is the answer to climate change. A technological solution like this is very much a last resort."

Dr Yusuf Hamied.

Matthew Greenig (Clare Hall)

Sormanni group

Matt was in the first cohort of Hamied Scholars in 2021 and became Dr Pietro Sormanni's first group member. His project is on a completely different scale from Daniel's.

With his background in Computational Biology, Matt was interested in Pietro's research developing new data-driven technologies for antibody design.

"As a biologist I had learned a lot about immunity, and I was fascinated by the idea that we could design antibodies and improve what the immune system has given us," he says.

Currently, identifying new drugs that can treat a given disease involves screening a large number of different antibodies and identifying the best candidates through trial and error. Matt wants to try something new and create computational models which will allow researchers to actually design the molecule they need.

He works with antibodies because they are known for their ability to attach to a diverse variety of molecular targets, which makes them promising for potential drug therapies.

He says: "We want to go beyond screening molecular candidates to designing antibodies for a particular purpose. My goal is to be able to design an antibody on the computer, then synthesise it in the lab and be confident that it will achieve what you want it to achieve."

Matt, who is now in his third year, says: "The idea of this project is to develop a methodology that can be applied to a wide array of protein targets. We've had some promising results in our computer models, but the only way to know whether they work now is to start testing out the models with real experiments in the lab."

Matt feels a responsibility about living up to being a Hamied Scholar. "Knowing Dr Hamied's name is associated with my funding is a big responsibility. It's a call to action and puts into perspective the meaning and the importance of the work we're doing here."

Other Hamied Scholars

2022

Jack Entwistle (Pembroke)
Knowles group (one year)

Siobhan Johnson (Magdalene)
Giorio group

Elisabeth Jones (Jesus)
Bernardes group

Papa Kwakye Kwarteng (Churchill)
Reisner group

Ilija Srpak (St Catharine's)
Althorpe group

Matthew Wheeler (Pembroke)
Barker/Boss group

2023

Wei Ting Khaw (Girton)
Bernardes group

Daniel Heraghty (Gonville & Caius)
Klenerman group

Tianyi Yang (Girton)
Spring group

Choy Boy (Girton)
Wales group

Learning from each other


Mercy Badu (left) and Melinda Duer.

Dr Mercy Badu is a Senior Lecturer in Chemistry at Kwame Nkrumah University of Science and Technology in Ghana, who researches the medicinal and nutritional properties of native plants. She and Professor Melinda Duer first met through a mentoring programme just before Covid hit. They are still learning from each other.

Melinda
We met through a mentoring programme sponsored and organised by the African Research Excellence Fund and other groups. The scheme officially concluded at the end of 2020, but we've kept connected because we have learned so much from each other. And I was delighted when Mercy was funded to work in our labs this summer through the Cambridge-Africa ALBORADA programme.

Mercy
There are many plants that grow wild in Ghana and my goal as a scientist is to find out if they have nutritional value or medicinal uses. If they do, no intervention would be needed other than to encourage local people to cultivate them. I work in savannah regions which are being affected by climate change, but these plants grow there and are not affected by weather variations.

Last year we collected many different samples and took extractions of several compounds. I fell in love working with the indigenous communities in Ghana, who use many of these plants. I felt there is a huge problem that needed to be solved – there is poverty, hunger and malnutrition.

What we need to know is whether these seeds have valuable nutrients, and how can our system best absorb and utilise them? In Cambridge we have been able to use NMR and mass spectrometry to correctly identify the compounds we have in these samples. Of course, we have basic instruments in Ghana, but yours are more advanced and we can determine molecular structures relevant to medicine and nutrition.

Melinda
Mercy brought along seven different types of plant tissues and seeds to look at, and we are helping with the interpretation of Mercy's NMR results, because they are really complicated, so everyone is pitching in. It's really collaborative support, and for us we are learning to understand better her scientific questions: eg, how are the plant oils locked up, what are they bound to, and what can we suggest to unbind them?

Mercy
For example, Baobab, which grows wild in Ghana, has been used as a traditional remedy for wound healing. Much of the plant is used, including the fruit and the leaves, but the seeds are left as waste. Some people have been trying to extract oils from the seeds for industrial products or skin or hair products, so we decided to look at the seeds and find out if they have nutritional value or possible medicinal uses.

I also brought along a seed of a melon that is popular in Ghana and grows very well in the communities where I do my studies. It is similar to peanuts and so is rich in oils. The problem is that the seed has a very hard husk so processing is difficult, but if we can process it, it has high nutritional value. I've also brought the desert date, which is not as succulent as Indian date. The local communities use the seed to feed animals but don't eat the seed itself.

I keep telling myself I have to get everything I want while I am here.

Melinda
No, you have to come back!

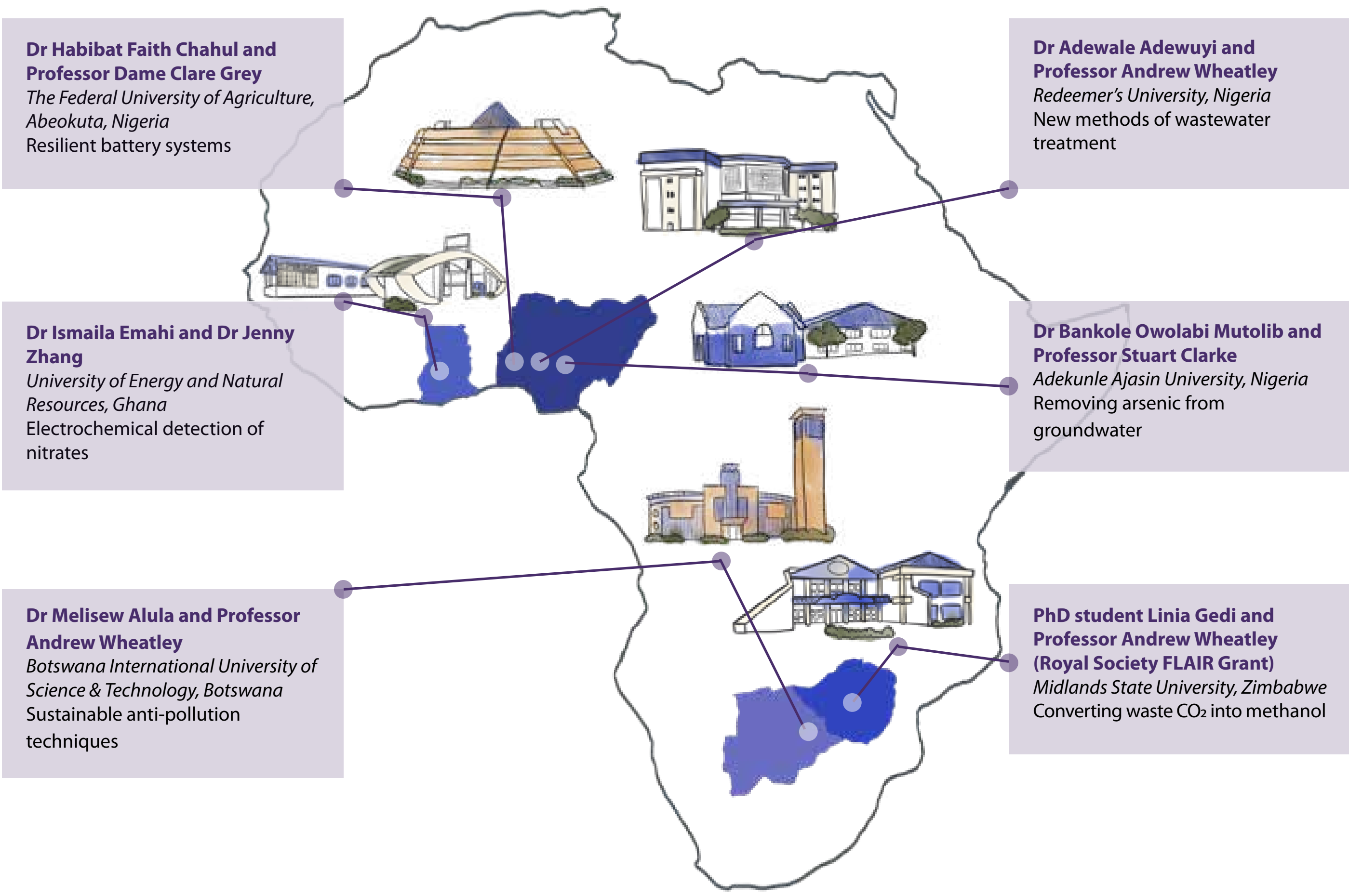
We are learning so much from Mercy. We have a huge drive in Cambridge to improve diversity in our undergraduate and graduate communities, but if you see what Mercy has done in Ghana, we haven't even scratched the surface.

Mercy
As part of my job with KNUST University, I work with women in STEM. Our slogan is "together we inspire generations." We provoke the interest of the young ladies in the local communities to pursue programmes in STEM. We go to local communities, and we look for underprivileged high schools where we offer science programmes during events like the International Day for Women and Girls in Science. In the long term, we plan to visit schools in rural communities with labs in a mobile van. And we bring up to 350 participants to our labs every year for a one-week intensive look at what science can do. We talk to the women about the importance of education to their girls. Some of these young women later become students in my department and it gives me a lot of pleasure when they greet me and tell me how they were inspired to study science from the courses we ran. But a lot still has to be done.

Melinda
It has been really good to work with Mercy. We give mutual support and bounce research ideas off each other – we all have different ways of approaching scientific questions, but we all face the same problems whatever the career stage. It's humbling to recognise there's a whole continent doing science and we don't hear from them because they don't have sufficient resources – we can help by giving access to our equipment. This gives enough data to help get bigger grants and write papers, but of course it doesn't solve the long term issues.

The Cambridge-Africa connection

The University's Cambridge-Africa programme supports African PhD and postdoctoral fellows and promotes collaborations and partnerships between Africa and Cambridge. A number of our research groups have hosted African scientists through its ALBORADA research fund and other schemes. *See the map for more details.*



Gates scholar pioneers graphene carbon capture

First year PhD student IniOluwa Afolabi (top right) is finding ways to manage the impact of climate change. She is supported by a Gates Cambridge Scholarship which is awarded to outstanding students from outside the UK who are commited to improving the lives of others.

Carbon dioxide (CO_2) is a harmful greenhouse gas and the major driver of climate change. As harmful as this gas is, it is also useful in fuel production and other major industrial synthesis. IniOluwa's goal is to reduce carbon emissions from sectors which so far have not seen much improvement due to technical challenges.

IniOluwa is working to identify materials that trap CO_2 on their surfaces. This gas can then be recycled into other useful chemicals or disposed of responsibly so that it does not affect the atmosphere. This process is known as carbon capture.

IniOluwa, who is a member of Professor Angelos Michaelides' ICE group says: "If there is anything I should be doing, it is mitigating the impact of climate change. This is part of what makes my group a great place to do my PhD."

Carbon capture with graphene

She searches for different materials that can be used for carbon capture. Graphene, a thin carbon material, is a good candidate because it is both accessible and its structure can trap gas molecules on the surface.

"Questions we need to understand are: 'How does CO_2 behave on graphene?'" says IniOluwa, "Then we can start asking 'Can CO_2 be turned into a different chemical on this surface' and 'how is that product useful industrially and economically?'"

However, CO_2 binds too weakly on graphene for meaningful CO_2 capture, so the surface must be altered to improve its strength. IniOluwa is testing graphene with different metals to figure out which coatings improve the adsorption strength.

Their first experiments have shown that certain metals improve graphene's ability to trap gases on its surface which is promising. They have also seen oxalates forming on the surface for the first time.

This work is part of the research that IniOluwa started in Angelos' group as a Mastercard Foundation Scholar at Churchill College. This programme provides fully-funded Master's degrees for students from under-represented communities in Africa.

Sustainable research

IniOluwa's work builds on ideas she developed in her earlier studies at the Ladoke Akintola University of Technology, Nigeria, where she researched wastewater treatment using activated carbon prepared from low-cost agricultural waste. Part of her research involved using coconut husks to remove ibuprofen contaminants from water safely and cheaply.

The coconut husk was first activated to open up small pores on its surface. These pores could then capture ibuprofen molecules in the waste water.

This promising research showed that the activated coconut husk is a viable and sustainable solution to clearing ibuprofen from water, and has potential for other pollutants. There are lots of applications for this research since waste products of many varieties end up in water, such as skin care, medications and pesticides.

Sustainable practices have led IniOluwa's research journey, and the Michaelides group is the perfect environment to continue addressing these challenges.

Angelos says: "We're very excited to have IniOluwa in our research group and looking forward to what comes from her research."

Gates Scholars

The Gates Cambridge Scholarship programme was established in 2000 with an historic donation of $210M from the Bill and Melinda Gates Foundation to the University of Cambridge. Each year Gates Cambridge offers around 80 full-cost scholarships to outstanding applicants from countries outside the UK to pursue a postgraduate degree. The Trust has awarded over 2,000 scholarships to students from more than 100 countries. These are the other Gates Cambridge scholars starting their chemistry PhDs in the department in 2023.

Sabrina Hu

Nitschke group
Queens' College
Synthesising supramolecular cages for climate change mitigation and adaptation

"I found myself drawn to chemistry not only because of its unique way of understanding our world, but also because of its unmatched ability to drive technological innovation, better the lives of others and protect our natural environment."

Kristen Burgess

Duer group
St Catharine's College
Researching the effects pancreatic ductal adenocarcinoma cells have on surrounding cells and tissue

"Once the mechanism of the disease has been mapped out, an intelligent molecular intervention can be designed. I am just delighted about what this opportunity has to offer me in my quest for knowledge, filling a research gap, sharing my love for science and combating this devastating disease."

Diksha Dewan

Wales group
Hughes Hall
Computationally analysing peptide staples for new treatments.

"I will work under the supervision of Professor David Wales and use energy landscape exploration methods to analyse stapled peptides, which possess the potential to be used as novel therapeutics for aberrant protein-protein interactions and in the treatment of cancer, cardiovascular and infectious diseases."

The green smiley face sticker is complete when the fume sash is closed.

Journeying toward sustainable chemistry

The department's sustainability committee is working together to reduce our carbon footprint.

Chloe Balhatchet, a second-year PhD student in the Forse group, has been the driving force behind setting up the committee and enlisting departmental support. Chloe is actively involved in sustainability programmes in the department, her college and the University, and earlier this year was awarded the Vice-Chancellor's Social Impact Award in Sustainability for her activities.

Over 22 department members attended the committee's first meeting in July, where they discussed a wide range of potential actions to improve sustainability within the department. These included continuing to improve the Nitrile glove recycling scheme, encouraging group members to shut the sashes on fume hoods, and asking research groups to adopt the LEAF scheme (Laboratory Efficiency Assessment Framework), which helps labs take steps to be more sustainable and efficient.

Support Services Manager Marita Walsh says: "By its very nature, a chemistry department has very large energy needs, from the use of fume hoods and strict ventilation rules to keep researchers safe, to the need to keep cell samples at constant temperatures. Over the past decade we have made great strides in improving efficiency, such as the introduction of the Wind responsive system in 2017 and the LED light replacements currently taking place. We will continue to strive to reduce electricity consumption where the opportunity presents itself."

Marita notes: "There are many steps individuals can take to reduce plug load, which is one of the main energy uses that we can control in the department. This includes sharing electrical equipment where possible to maximise its capacity, and turning it off when it isn't needed."

The group ran its first Green Week at the beginning of November in which they encouraged researchers to "Shut the Sash" to reduce energy consumption in the department. To encourage students and researchers to reduce plug load, the committee has created happy face labels which form a smile when a fume hood is closed.

They also scheduled a drop-in session to hear from Merck on their sustainability goals, screened the film *I am Greta* about Greta Thunberg (followed by plant-based pizza), and hosted a panel event which included speakers Dr Chris Macdonald, author of *Operation sustainable human*, and Dr Sara Lightowlers, a campaigner for the Mothers' Climate Action Network and Cambridgeshire Parents for Sustainable Travel and Plant-based Councils.

Chloe says: "48 people are now members of the Chemistry Sustainability Teams channel, and we hope to see this community continuing to grow."

Behind the scenes in... Housekeeping

Meet Eve Lechowska, who took up the newly-created role of Housekeeping Manager at the end of July. Eve manages the department's cleaning staff and is responsible for housekeeping and the Cybercafe's operations. She also helps out in Reception.

Colleges and Departments

I used to work in Christ's College where Yusuf Hamied was a student, and where he has also generously given funds for many buildings and projects. Working in a college is quite different from working in a department – although the job is the same, the environment is completely different. Here, it's labs and offices, while in college you have student accommodation, and you see the students more often.

Challenges

The biggest challenge for me in starting this job was first of all meeting all the people, and also getting to learn how the place operates. Colleges and university departments are different, so it was important to learn how everything works – what makes it 'tick'.

A people person

Definitely the best thing about my new role is working with people, I like to talk with people and listen to them as well – it's always good to talk.

What would surprise people about you?

I am a massive K-Pop fan. It started when I was watching Japanese dramas (I love Japan-related things), which got me into Korean dramas, and then I started to listen to the music. K-Pop is not just BTS, although I do know their songs and occasionally add them to my playlists. (Note for readers: K-pop stands for pop music from South Korea, and BTS is one of the most popular K-Pop boy bands!)

Coffee or tea?

Coffee definitely. Possibly controversially, I prefer Starbucks.

Gifts fund summer projects

Once again this summer, Wyn Lewis-Bevan (Churchill 1979) and our Chemistry@Cambridge Opportunity Fund have supported four undergrads to experience what it's like to complete a project in a research group. Two of them report on their experience.

Jonah Eicke

Jonah (Trinity Hall) completed an eight-week summer internship in Professor Matthew Gaunt's synthetic chemistry group, funded by the Chemistry@Cambridge Opportunity fund. He is now completing his Part III project in the Gaunt group, working on guanosine functionalisation.

During Part II Chemistry, I was thinking about applying for a PhD, but I didn't know for sure, so a summer internship was a good way to try it out. I had developed an interest in synthetic chemistry and I wanted the chance to get some experience in the lab, so I applied to Prof Gaunt's group.

I worked with Dr Abigail Barker-Mountford on the synthesis of a molecule called cGAMP, which plays a role in the natural immune response. The group has a partnership with a group at Addenbrooke's to test modified versions of cGAMP, but before you can modify it you have to make some!

I think the biggest thing I learned was developing practical, useful chemistry skills. I am already using them for my Part III and I will need them for a PhD. I also learned a lot from seeing how people went about their research. It was different from lectures and supervisions and practicals; I had a supervisor but was also working for myself, on my own ideas.

I enjoyed my time going into the lab. I thought 'I could do this for four years' so I'm now applying for PhD programmes. I'd like to thank the funders of the internship: They've provided me with a really brilliant opportunity, and I am grateful.

This fund also supported Harveen Kaur's project in Professor Angelos Michaelides' ICE group.

Amber Wright

Amber (Trinity) was funded by Wyn Lewis-Bevan for her project in Professor Stuart Clarke's surface science group. She is now looking at Master's programmes in physical chemistry.

I was doing my Part II in Chemistry and I wanted to get some lab experience and a feel for what it might be like to do a PhD. I like physical chemistry so I chose a project on battery electrolytes.

To develop new and better electrolytes for batteries, we need to know how they behave in solution. I was looking at their freezing point depression, which is the principle we see when we put salt on roads in cold weather to prevent ice formation. This occurs when we add any solute to any solvent. If we can precisely measure the amount the freezing point changes after doing this, then we gain information about the electrolyte. Our hope is that this method will provide a quicker alternative to DFT (density functional theory) calculations.

I learned a lot during my internship about how projects run: I made bumpy progress and the technique didn't work particularly well, so I think it gave me a more realistic view of research. I also became much more interested in the practical applications of research, and now I am looking for a Master's with sustainable applications.

I would like to say thank you very much to Wyn Lewis-Bevan. I really enjoyed the project, I loved working in a collaborative lab environment, and to feel so supported and capable whilst doing the project made me very excited about my future career.

This fund also supported Iona Lynn's project with Dr Mike Casford.

A battery of FUSE interns

Undergrad Daniel Leong completed a summer project in the Grey Lab and won a prize for his research poster.

Daniel's summer project was funded through the Faraday Undergraduate Summer Experience (FUSE), which funds up to 55 undergrads a year to complete eight-week paid placements in battery research.

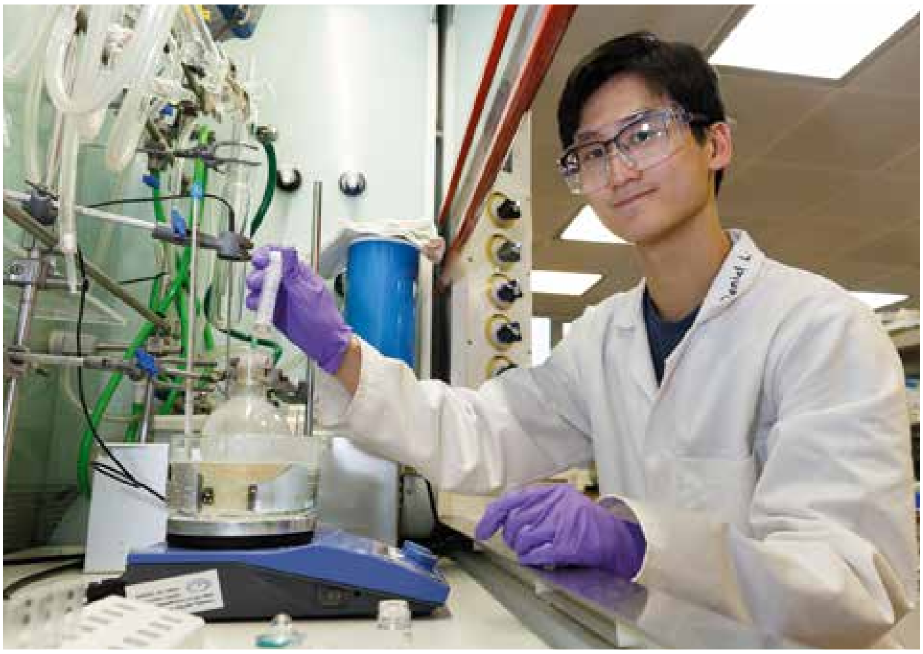
The Faraday Institution is the UK's flagship battery research programme. "We have a real shortage of people in the UK going into science, engineering, technology and maths, and we needed to come up with innovative ways to attract people and diversify the pool of talent going into the battery sector," says Dominic Grantley-Smith, who manages FUSE.

"I think FUSE is a fantastic programme. There aren't many internships where undergrads get the experience of being embedded in a research group and to add their research directly to the field."

FUSE

Daniel says: "My research interests have always centred around sustainable chemistry and climate science. I've done electrocatalysis, photocatalysis and carbon capture. But I had never done battery research – it felt really complicated, but after reading the project descriptions I thought I could contribute something."

Daniel was one of six interns selected to join Professor Dame Clare Grey's group for the summer, where he and his supervisor, Dr Israel Temprano, researched ways to improve the performance of Lithium Air (Li-air) batteries. Daniel says he learned a lot, especially when things didn't go as planned. "By week three Israel and I realised that the material we were using was very restricted in its performance, but creating a new material wasn't possible in the time we had. I learned how to embrace the uncertainties of research, and we pivoted to a different research direction."



Great Communication

The FUSE programme requires students to produce a poster which summarises their research and results. Daniel's prize-winning poster was recognised for 'skilfully taking a difficult to understand aspect of batteries and explaining it very clearly in a way that is accessible across the field. The technical communication is high-quality, with the process and methodology clearly expressed.'

Israel says: "The poster award was totally deserved, as Daniel mastered a very complex subject with ease and demonstrated a great aptitude for research."

Part III

Daniel is now completing his Part III project in the Reisner group, where he is researching strategies to improve sustainable, sunlight-driven CO_2 conversion.

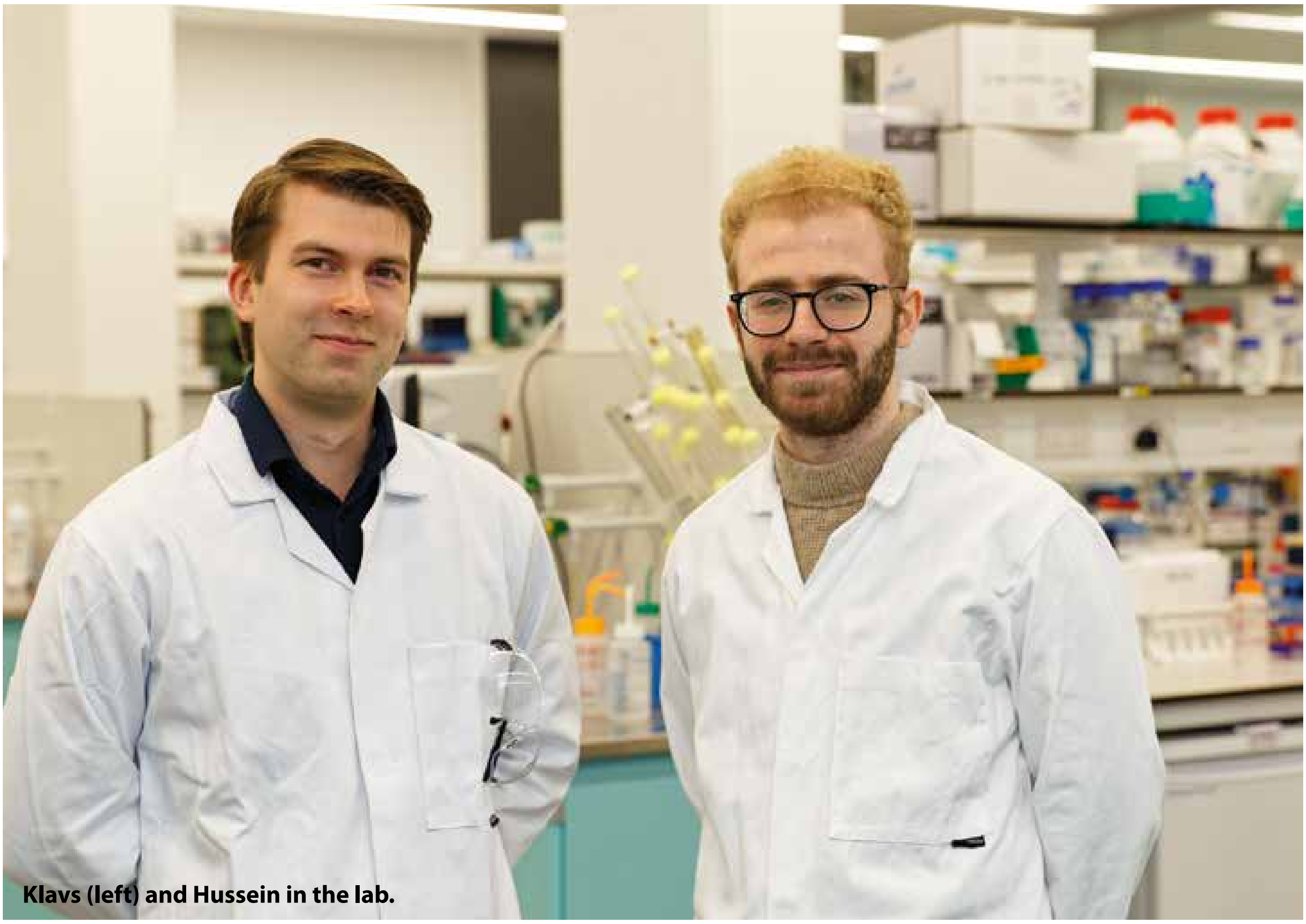
"I've always wanted to do research in CO_2 reduction ever since my first research experience in high school, so I've somewhat come full circle. We are facing a climate crisis and we need to drastically reduce our emissions, but there are some emissions we can't remove in the near term. Carbon capture and conversion are essential to allow us to hit our net zero targets."

Other FUSE summer interns

William Metcalf, supervised by Dr Farheen Sayed; Tom Lancaster, supervised by Dr Marie Juramy and Dr Svetlana Menkin; Aditya Varshney, supervised by Dr Hrishit Banerjee; Luke Rasmussen, supervised by Dr Samuel Niblett; and Laurence Wells, supervised by Dr Veronica Sedajova, Dr James Simon and Dr Svetlana Menkin.

Finlay scholars search for Parkinson's treatments

Mr R Derek Finlay (Emmanuel 1952) founded the Una Finlay laboratory in 2016 in memory of his wife, who passed away from Alzheimer's disease. A further gift last year will support a number of postgraduate studentships, hosted by Emmanuel College. Meet our first two Una Finlay scholars, who started in October.



Klavs (left) and Hussein in the lab.

Hussein Murtada

Vendruscolo Group

Hussein discovered some promising small molecule drug candidates for Parkinson's disease during his Master's degree with the Vendruscolo group in 2022. He is tackling a more intricate issue for his PhD: the identification of drug candidates capable of binding to disordered proteins.

This is highly relevant in neurodegenerative disorders like Alzheimer's and Parkinson's, certain proteins misfold and aggregate, contributing to disease progression. Typically, proteins fold into stable states with pockets, and drugs are designed so that they fit into these pockets akin to a lock and key mechanism.

In contrast, disordered proteins have dynamic and unpredictable structures, lacking a reliable 'pocket.' Diseases like Alzheimer's can arise when these proteins undergo misfolding, posing challenges for developing treatments.

Currently, there are no widely available treatments for Alzheimer's or other diseases associated with disordered proteins. However, Hussein's research aims to simulate the behaviour of these proteins by writing software that uses machine learning and molecular dynamics. He hopes to identify small molecules that will bind to the computer model that could be potential drug candidates. A drug candidate for this challenging protein would represent a significant advancement in the field of molecular pharmacology.

This is based on the 'disordered binding' mechanism discovered in the Vendruscolo Lab, paving the way for potential breakthroughs in developing effective therapies for neurodegenerative diseases.

Hussein comments: "I am optimistic that our research could unlock numerous avenues for groundbreaking drug discovery. By delving into the realm of disordered proteins, we aim to uncover potential treatments for diseases that currently lack effective therapies. My aspiration is that this work will create a significant impact, offering hope and new possibilities for patients and researchers alike."

Klavs Jermakovs

Knowles lab

'You can't see the forest for the trees' means missing out on the overall picture by focusing on the small details. To avoid this, Klavs takes a bird's eye view approach to proteins by assessing how millions of different protein variants behave and tries to unravel why some generally misbehave.

The field of neurodegenerative disease research needs large datasets that describe the diversity of disordered proteins. In particular, Klavs wants to build these datasets and focus on protein aggregates that are formed in diseases such as Parkinson's disease. His hope is that, with his datasets, it will be possible to find the fundamental mechanisms of protein misbehaviour.

"The purpose of examining proteins and how they interact on the large scale is to observe patterns that would otherwise be hidden," he explains.

Klavs uses an unusual hybrid of computational models and laboratory data in his research. He tests large numbers of compounds and uses the results in tandem with computational methods to unravel the rules that govern protein misfolding and aggregate formation.

Klavs comments: "I'm excited to do research on the interface between computational and experimental methods. My belief is that by combining the two it is possible to solve questions that previously have been out of reach."

One of the proteins he aims to study during his PhD is alpha synuclein, which is the disordered protein that malfunctions in Parkinson's disease. The protein forms aggregates which damage pathways in the brain.

This data-driven research carries on from work that Klavs started during a six-month internship in Tuomas Knowles' laboratory in 2022 while completing a Master's degree at the University of Tartu, Estonia.

Spinout Update

TargTex, founded by Professor Gonçalo Bernardes, has been awarded €14M from the European Innovation Council Accelerator fund to proceed with clinical validation of its implantable scaffold/hydrogel anti-cancer therapy. TargTex is developing targeted therapies for glioblastoma multiforme, based on his group's research into the natural anticancer agent piperlongumine.

Dr Andreas Bender is heading up **PangeAI**, the computational arm of Pangea Bio, which uses natural products from plants with a history of traditional use to improve the chances of success in clinical trials for treating diseases of the central nervous system.

Grey group spinout **Nyobolt** has partnered with Lotus Elise designer Julian Thomson and engineering business CALLUM to design and produce a concept electric vehicle which can charge fully and repeatedly in less than six minutes – a new record in automotive electrification.

Bender group alumna Dr Layla Hosseini has co-founded and is Chief Data Science Officer of **Ignota Labs**, whose AI platform can predict, understand and solve safety problems that may occur in the drug discovery pipeline.

PharmEnable, a spinout from the Spring and Bender groups, closed a £7.5M Pre-Series A financing round led by MP Health care, the venture arm of Mitsubishi Tanabe Pharma group, to develop the next generation of small molecule drugs to treat cancer and neurological diseases. PharmEnable's drug discovery platform can predict improved small molecule hits to targets across a range of disease areas.

Alumnus recognised for drug discovery research

Kelly Chibale (Queens' 1989), who completed his PhD in synthetic organic chemistry with Stuart Warren, already has a string of honours and awards to his name and he's just received two more.

Kelly is Professor of Organic Chemistry and holds the Neville Isdell Chair in African-centric Drug Discovery and Development at the University of Cape Town (UCT). He is also the founder and Director of UCT's ground-breaking Holistic Drug Discovery and Development Centre (H3D), one of only a handful of integrated drug discovery centres world-wide embedded within an academic institution.

Royal Society Africa Prize

In August, Kelly was awarded the Royal Society Africa Prize for his exceptional leadership and groundbreaking research in African endemic diseases. Kelly's synthetic organic chemistry and drug discovery research at UCT focuses on malaria, tuberculosis and antibiotic-resistant microbial diseases. But when Kelly moved to UCT in 1996, he soon discovered a problem – the researchers had limited translational research infrastructure and technology platforms. "I realised that I needed to also work on using science for development, meaning scientific entrepreneurship, to create capacity to attract, develop and retain talent in Africa," he says.

"This is why I founded H3D in 2010, which brings together all the disciplines you need to move a project from the lab to the clinic. We had to build the infrastructure and technologies from scratch, and also build a critical mass of talent. We now have an integrated, world-class centre. I feel

[1]G. Turon, J. Hlozek, J.G. Woodland, A. Kumar, K. Chibale, M. Duran-Frigola, *First fully-automated AI/ML virtual screening cascade implemented at a drug discovery centre in Africa, Nature Commun,* (2023) 14,

very proud about my leadership of H3D, which has grown from five to 76 people."

H3D was selected by Johnson & Johnson last year as one of three J&J Centres for Global Health Discovery worldwide (the other two are in London and Singapore). Kelly still maintains his separate and independent academic group training PhD students and postdocs.

Another strand of Kelly's research is to develop tools and models to improve treatment outcomes in people of African heritage. "We want to address the longstanding problem of sub-optimal efficacy and safety of medicines used in Africa," he says. "The African population is the most genetically diverse on the planet, but most clinical trials still use northern European males."

"We have to consider the African perspective in terms of intrinsic factors like our physiology and genetics, but also extrinsic factors, like the ways Africans practise medicine. For example, at what stage in an illness they go to the doctor, which is usually quite a bit later in Africa. There are also many co-morbidities, which complicate matters."

Artificial Intelligence 2050 Senior Fellow

In October, Kelly was one of seven scientists selected as Artificial Intelligence 2050 (AI2050) Senior Fellows by the philanthropic organisation Schmidt Futures. The honour recognises established leaders who are working on ways to increase the beneficial promise of AI.

AI2050 fellows receive a two-year award to work on specific projects that use artificial intelligence for the benefit of society. This is particularly valuable in Africa, according to Kelly, who recently published a paper in *Nature Communications* which demonstrates how AI can fast track progress in resource-limited settings.

He was also one of 15 global leaders in drug discovery brought together by the Wellcome Trust to inform the Boston Consulting Group landscaping report *Unlocking the potential of AI in drug discovery.*

"Most of Africa doesn't have the infrastructure we have here in UCT, and AI presents a real opportunity with its potential to speed up the process. In some cases, you don't need very sophisticated computational infrastructure to use AI to meaningfully participate in drug discovery."

It all started in Cambridge

Kelly remains eternally grateful to Stuart Warren for the guidance he gave when Kelly arrived from Zambia for his PhD. "I was very disadvantaged and very ill prepared; everything was completely unfamiliar. But Stuart was such an incredible teacher. If you consider the size of his group and how many people have gone into academia, it's remarkable. Stuart laid the foundation for the person I am today professionally. His intellectual ability raised the bar and standard for me to aspire to."

Kelly, who himself came to Cambridge on a scholarship, played a key role in setting up the Stuart Warren Studentship, which provides a place at Churchill College for a PhD student from Africa to study chemistry.

The first holder of the studentship, Choonzo Chiyumba, started here last year and is designing artificial metalloenzymes that can act as catalysts (see Chem@Cam Spring 2023 Issue 66). "I had nothing to do with her being selected, but it's remarkable that Choonzo is also from Zambia, where I came from." What goes around comes around.

Kelly in his student days at the department, above and top left.

Introducing our new group leaders

Join us in welcoming the five new group leaders in the department. Find out who they are, their research, and their plans for their groups.

Dr Mateo Isidro Sanchez Lopez

Wellcome Trust Fellow

Mateo works at the frontiers between chemistry and biology, developing new molecular tools for cell biology and neuroscience. He completed his PhD in organic chemistry in Spain and the focus of his thesis was on DNA recognition by designed fluorescent binders. As he was eager to learn molecular biology and directed evolution, in 2015 he joined the group of Prof Alice Ting at the Massachusetts Institute of Technology (MIT), and later the Department of Genetics at Stanford University with an EMBO long-term postdoctoral fellowship. Mateo most recently held a Marie Curie Fellowship at Imperial College London, where he designed genetic circuits to study DNA repair mechanisms.

With his own research group in the department, Mateo plans to continue research into the mapping and manipulation of active neuronal circuits underlying specific behaviours, by developing new molecular tools.

Additionally, he is designing enzymes that can be used to make small molecules used in pharmaceuticals. He adds: "My goal is to use enzymes to make small molecules that would be very difficult to obtain by traditional methods. These molecules could be more affordable building blocks to make complex drugs."

Dr Svetlana Menkin

Royal Society University Research Fellow

Previously in the Grey Group, Svetlana's research interests cross the broad areas of electrified interfaces, energy storage materials, alkali and multivalent metal plating and surface electrochemistry. She studies the materials and electrified interfaces in batteries to make them more sustainable and safer. Batteries are made up of many different materials and interfaces and Svetlana's work looks at ions and electrons moving on an electrode's surface. The fundamental question she researches is how a charge moves across different interfaces. Recently, she expanded her research into understanding and preventing battery short-circuiting.

Before Svetlana joined the Grey group, she had industry experience developing high-energy electrodes for lithium batteries and supercapacitors. Now embarking on her own group, she is specifically looking for ways to replace rare and precious elements in batteries with more abundant and sustainable resources, such as sodium, calcium and aluminium. She comments: "I look forward to building a group that spans many disciplines of surface electrochemistry and battery research and collaborations so that we can develop tools that improve batteries across all stages."

Dr Pawel Dydio

Assistant Professor in Synthetic Organic Chemistry

Pawel's research focuses on discovering new strategies to make the synthesis of chemicals and materials clean and efficient, with the overarching aim to make the chemical industry sustainable.

Pawel says: "Catalysis is the key technology to meet the challenges of our society, especially in the context of the responsible use of resources, energy and waste mitigation. I think the real breakthroughs can be triggered by the detailed understanding of catalytic processes at their core." Therefore, a large part of his research programme at the department is dedicated to studying and improving catalytic reactions, especially where there are no available alternatives.

Although the research is primarily curiosity-driven, it may soon lead to innovations of practical significance. For instance, the group has recently addressed a long-standing issue in industrially-relevant hydroformylation processes. Pawel is collaborating with an industrial partner to bring this technology to the market.

Dr Ruth Webster

Assistant Professor in Synthetic Organic Chemistry

Ruth aims to design sustainable catalysts to bind elements together more efficiently. Catalysts help enable reactions that would normally require a lot of energy, but many metals used as catalysts are in everyday objects such as our mobile phones. Ruth aims to replace these precious metal catalysts, such as palladium or rhodium, with a more sustainable alternative: iron. Her research focuses on understanding how iron can act as a catalyst and how to make it act more like a precious metal.

Ruth comments: "Iron is not a simple drop-in replacement for the precious metals, unfortunately, so we need to understand how iron works in catalysis."

She uses many different spectroscopic, spectrometric and computational techniques to investigate how catalysts work on a molecular level. Her work at the department will build on her catalyst research which began in 2014, when she used iron as a catalyst to promote a phosphine reaction. Her research can help make chemical production more sustainable, such as in the case of phosphine products which are used in pharmaceuticals and agrochemicals.

Dr Julian Willis

Assistant Professor in Chemical Biology

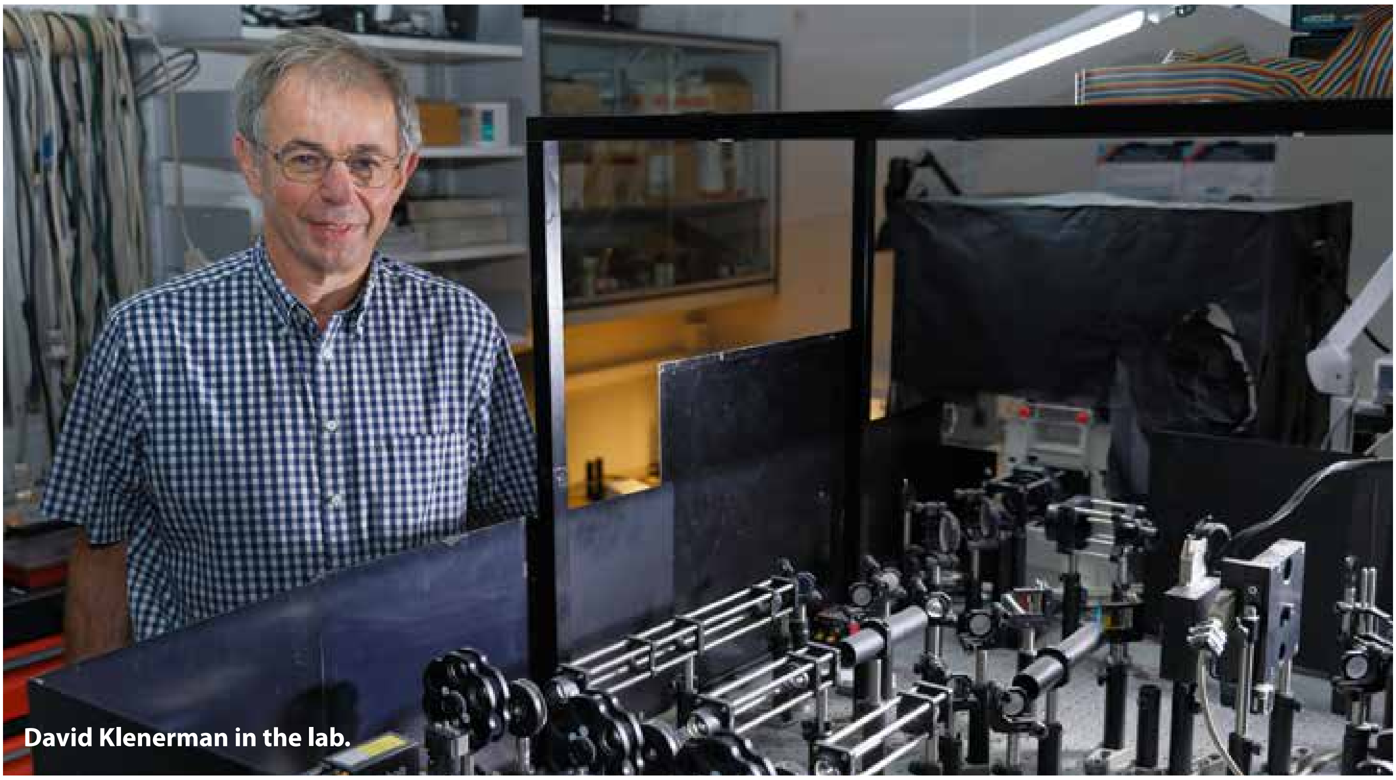
Julian joins the department after completing his postdoctoral work where he designed new proteins which were able to correct mutations in our genetic code. This work was done in MIT and Harvard at the Broad Institute in Massachusetts, a multidisciplinary genomic medicine research organisation.

Julian now studies, characterises and engineers an unusual class of virus which has the potential to be harnessed for treating genetic diseases. These viruses have an intriguing mode of replicating themselves, with the unique feature of a viral protein that remains permanently attached to their DNA. Julian is investigating this unusual replication process so that it can be repurposed as a tool for gene editing to treat genetic disease.

"Because this sort of gene editing is so new there are still lots of challenges to overcome. We have huge databases of genes from bacteria and viruses found in the soils or oceans with untapped potential. Now we need someone to look through them and find new tools. I'd like to make a dedicated effort in this search."

New biomarker for Parkinson's disease

Researchers in the Klenerman group have developed a new biomarker for Parkinson's disease that paves the way to an early-diagnosis blood test and more effective treatment.



David Klenerman in the lab.

Scientists have long known that clumps of misfolded proteins, called aggregates, accumulate in the brains of people who suffer from neurodegenerative conditions such as Alzheimer's and Parkinson's diseases.

Aggregates of certain proteins, such as alpha-synuclein and beta-amyloid, are particularly associated with the development of Parkinson's disease (PD). For example, alpha-synuclein aggregates create deposits in the brain called Lewy bodies, which eventually lead to the destruction of dopamine neurons that is associated with the condition.

Early diagnosis

Currently PD can only be diagnosed after physical symptoms start to develop, at which point many dopamine neurons have already been lost. Earlier diagnosis would mean more effective treatments could be given at an earlier stage of the disease.

Yu Zhang, who worked on this project for his PhD, says: "You want to be able to diagnose way before someone develops symptoms of the disease, when treatment can be more effective. We believe our new method might be able to do this."

Too small

The problem until now has been the inability to easily and accurately measure the small amounts of aggregates in the blood and assess which characteristics will lead to Parkinson's disease. To overcome this, Professor Sir David Klenerman and his team developed a new combined method which allows them to 'fingerprint' the aggregates in easily prepared blood serum samples.

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[1]Y. P. Zhang, E. Lobanova, D. Emin, S. V. Lobanov, A. Kouli, C. H. Williams-Grey and D. Klenerman, *Imaging protein aggregates in Parkinson's disease Serum using Aptamer-Assisted Single-Molecule Pull-down, Analytical chemistry,* (2023) 95, 41, 15254 - 15263

A new technique

First the team used a highly sensitive and specific single-molecule imaging platform called single-molecule pull-down, through which they showed that the ratio of alpha-synuclein to beta-amyloid aggregates was higher in PD blood than control groups. They then used super resolution microscopy to measure the size and shape of the aggregates, and found that the aggregates in PD blood tended to be larger and rounder. They combined the two techniques to develop the biomarker.

David says: "Aggregates have been very challenging to study because they are at very low concentrations, and so selectively capturing them and measuring them in the blood is a real technical challenge. With our new tool we can measure size and shape and also identify different aggregates such as those of the Tau protein, which is also associated with Alzheimer's disease. There is no complex processing, we can simply dilute the serum sample and stick it on the slide. It's a technical tour de force."

A new biomarker

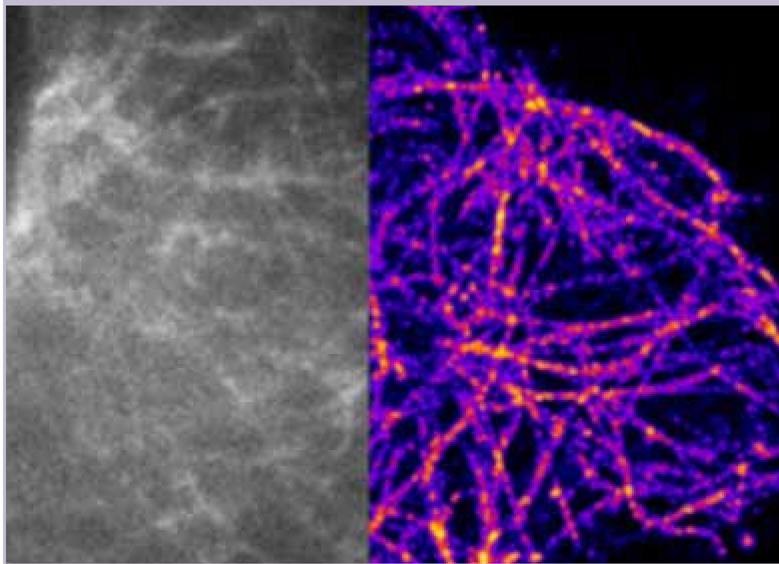
The researchers applied the new technique to human blood serum from patients who had been diagnosed with PD for no more than one year, and compared the results with samples from non-PD patients. They found that the ratio of alpha-synuclein aggregates to beta-amyloid aggregates was higher in the PD serum than in the control group. Additionally, the PD serum had a higher portion of larger and rounder a-syn aggregates than the controls. By combining these two metrics together they achieved a very high diagnostic accuracy.

Next steps

The combined technique is called APSiMPull. The researchers have recently been awarded a three-year MRC grant for £1M to continue their work. They believe the technique could also be used to find biomarkers in Alzheimer's and other neurodegenerative diseases.

"We are looking forward to continuing our strong collaboration with the clinicians Dr Caroline Williams-Grey and Professor James Rowe at the Cambridge Biomedical Campus," says David. "They are the ones who see the patients and provide insight, and they have been very generous in giving us the samples we need. We are also very grateful to the patients who have provided blood and lumbar samples."

Alzheimer's Disease



Images of soluble tau using conventional microscopy (left) and super resolution microscopy (right), courtesy Klenerman Lab.

In other work, the Klenerman group has also been able to observe and measure tau aggregates replicating in cells for the first time, in a key process that underpins the development of Alzheimer's disease.

The tau aggregates grow in an exponential fashion: this means that one fibril can grow longer, then break into two, which also grows and splits, and so on, much like the broken broom in the Disney version of *The Sorcerer's Apprentice*.

Co-first author Dr Eleni Dimou established the methodology to study the tau aggregation, using single-molecule localisation microscopy, a type of super resolution microscopy.[2]

"The microscopy allowed us to detect small aggregates at about ten times better resolution than before," explains Eleni. "We also were able to detect small aggregates at very early stages, within hours of seeding rather than days, which gives us a better understanding of how these early stages of tau aggregation occur."

Eleni, who is now a scientist at AstraZeneca, says: "I think it's exciting to be able to share this information with other scientists. I hope they will be able to use this new methodology to address their own scientific questions, and help the science to progress more quickly."

[2]E. Dimou, T. Katsinelos, G. Meisl, B.J. Tuck, S. Keeling, A.E. Smith, E. Hidari, J.Y.L. Lam, M. Burke, S. Lovestam, R. T. Ranasinghe, W.A. McEwan, D. Klenerman, *Super-resolution imaging unveils the self-replication of tau aggregates upon seeding, Cell Reports* (25 July 2023), Volume 42, Issue 7.

New way to alter proteins

Researchers in the Centre for Misfolding Diseases have developed a system to modify naturally occurring proteins in a biological environment for the first time, opening a path to new therapies for illnesses such as Alzheimer's disease and cancer.

A guided missile

The new system uses antibodies which bind to a specific site on the targeted protein. The antibody transports an attached 'linker' to the selected site, where it delivers a chemical payload which makes the desired modification.

One advantage of the new technique is that the payload has only a short-lived connection with the antibody and linker, and breaks away after it is delivered to the protein. The antibody and its attached linker are then cleared from the cell, which reduces the risk of adverse side effects.

Dr Oded Rimon, who started the project as a PhD student and is now a postdoctoral researcher in the Vendruscolo group, says: "The antibodies are essentially used like a guided missile – they find and bind to the protein and deliver their payload, which reacts with the target to make the modification."

Oded calls the system PEABS, which stands for Protein Editing with an Antibody-Based System. "All credit to my Dad, who came up with this acronym," he says. "It's a new approach to post-translational modification of proteins."

Modifying proteins

Post-translational modifications (PTMs) of proteins are chemical modifications that regulate a broad range of cell behaviours. They occur naturally and can happen at any step in the life cycle of a protein. Scientists like Oded have long been interested in finding ways to make their own post-translational modifications of proteins as a potential way to prevent or cure disease.

But finding a way to modify naturally occurring proteins in a complex biological environment has proved to be very difficult, and this is the first time scientists have shown they can create a desired modification on proteins in their natural state.

Potential applications

Oded is confident that his system could eventually be used as a therapy in neurodegenerative diseases. He foresees a day when the system could be used to modify the amyloid beta protein so that it doesn't aggregate, for example. The research has been uploaded to the preprint server *bioRxiv*, so that others can review the system. He has now submitted the paper for peer-review and publication.

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[1]Oded Rimon, Juraj Konc, Vaidehi Roy Chowdhury, Gonçalo J. L. Bernardes, Michele Vendruscolo, *Targeted protein editing with an antibody-based system, bioRxiv preprint server,* (2023)

Stable peptides for medical breakthroughs

Sona Krajcovicova, a postdoctoral research fellow in the Spring group, works on stabilising peptides for safe and stable drug delivery.

Peptides are flimsy strings of amino acids that Sona coils into a spring shape which is more resilient and stable so that they can survive inside the body. They have promising uses in medicine since they aren't toxic, are easy to make and are versatile.

Using a technique called peptide stapling, Sona punches molecular staples onto peptides to reinforce them and imbue them with a range of interesting properties. Staples can bear a variety of things such as drugs for medicine or fluorescent dyes for imaging. Their versatility makes these peptides attractive for designers.

Sona comments: "In our research, we are focusing primarily on finding new methods for making stapled peptides but there are lots of different applications for this technology. What is novel in our stapling approach is the use of the naturally occurring amino acid tryptophan with a multicomponent reaction sequence – a combination that has never really been shown before."

Punching staples

The key amino acid in Sona's research is tryptophan, an amino acid that can naturally be found in milk. Tryptophan's core has some unique properties; however, its use in peptide stapling has been limited. Sona's research is the first to bridge all of these aspects and establish a platform for synthesising a variety of peptides.

The new method can be easily customised to make a lot of different products using just one common intermediate. This saves money and time and therefore can have a high value for pharmaceutical use.

"Sona's transformational research will help to bring chemistry, biology and medicine closer together," comments Professor David Spring. "She is a pleasure to work with and I am so pleased all her hard work paid off."

Sona's research was published in *Angewandte Chemie International Edition*[1]. The article is the first time that Sona has been published as a corresponding author and she had a prestigious 'about the author' introduction as well. "Happy days, not gonna lie!" Sona says about the achievement.

Applications

Sona started her chemistry studies in the Czech Republic, doing her Master's at Masaryk University in Brno and finishing her PhD at Palacký University in Olomouc. Her pursuit of the next generation of therapeutics led her to Cambridge and the Spring group.

In her introduction, she comments on her journey into peptide research: "I have a vivid recollection of that exceptionally chilly December evening, which occurred shortly after my initial visit to Cambridge. I found myself at home, sipping tea and diligently crafting a proposal for my independent fellowships. Out of nowhere, the idea struck me like a bolt of lightning! I was immensely grateful when it received financial support, allowing me to delve deeper into the topic.

"Although I had anticipated the project to be challenging, it surprised me how stubborn and not-so-easily tamed peptides could be! Thankfully, perseverance paid off and I managed to achieve success in the end."

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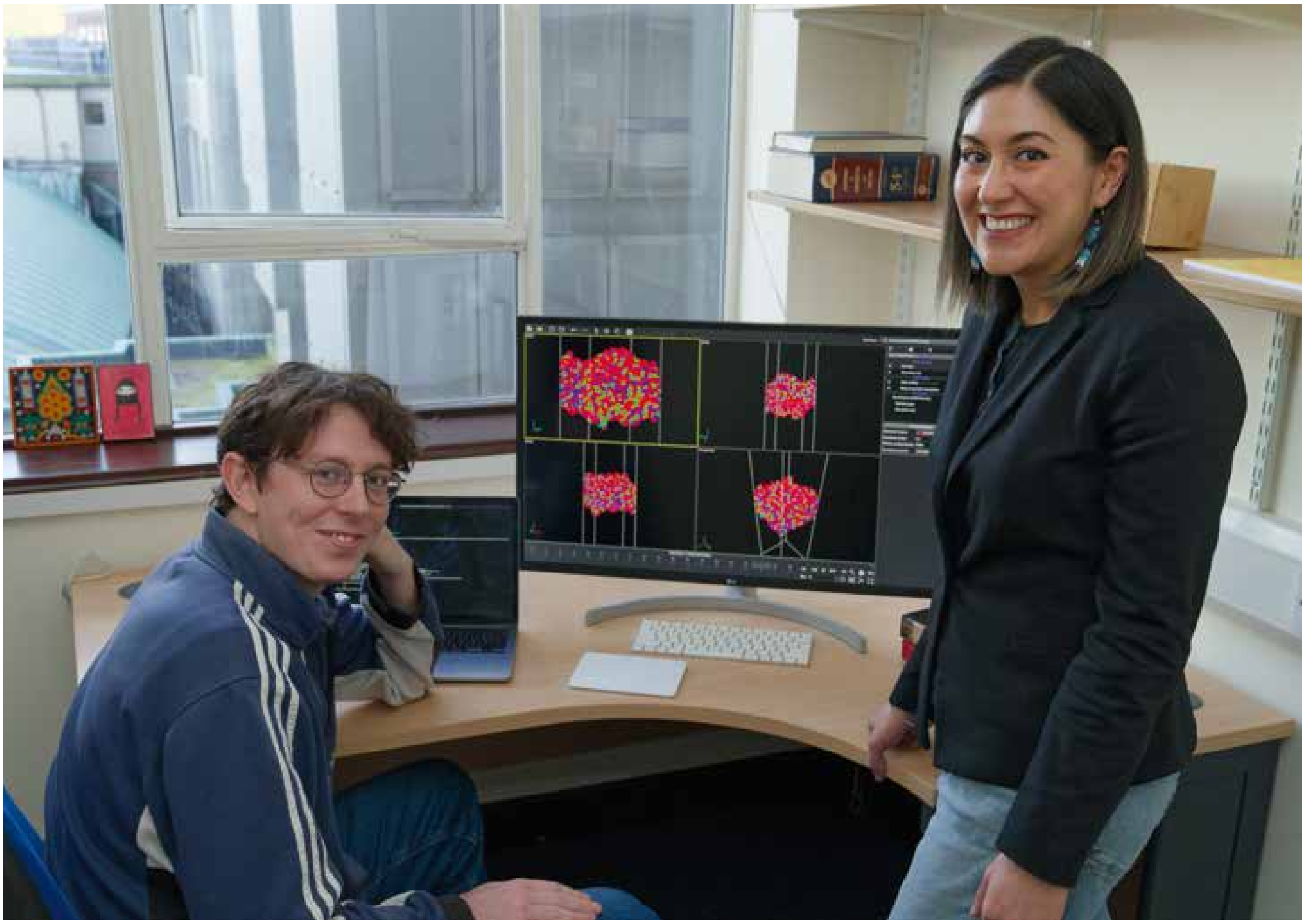
[1]Krajcovicova S, Spring DR. *Tryptophan in Multicomponent Petasis Reactions for Peptide Stapling and Late-Stage Functionalisation, Angewandte Chemie International Edition,* (2023) 62 34

Field trip unfolds DNA

Members of the Collepardo lab took part in a month-long 'Chromatin Consortium' to help unfold the mysteries of the material that makes up our chromosomes.



Kieran Russell and Rosana Collepardo with chromatin models.

Organising DNA

Chromatin is the structure inside our cell nuclei that organises DNA like knitting organises wool into a scarf. If a strand of DNA from a single cell were uncoiled into a straight line then the length would be two metres long. That is taller than most adults, yet the cell nucleus is only a few microns in diameter.

The intricate three-dimensional organisation of chromatin ensures that only specific parts of the DNA strand, ie specific genes, are expressed as required. For example, chromatin ensures that liver cells grow in the liver and brain cells grow in the brain.

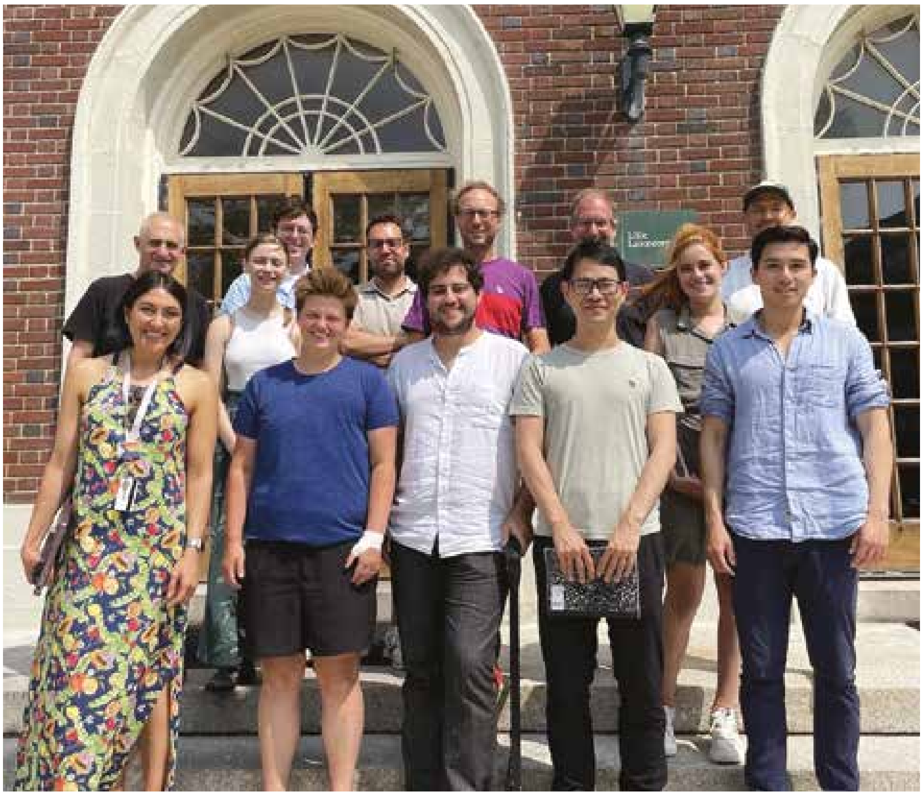
There are still many mysteries around how chromatin is organised inside cells. The Chromatin Consortium was designed to advance the understanding of chromatin organisation and behaviour.

Chromatin Consortium

The consortium brought together the research groups of Professor Mike Rosen and Professor Sy Redding from the USA, Professor Daniel Gerlich from Austria and Professor Collepardo from Cambridge to the Marine Biological Laboratory in Woods Hole, Massachusetts. The aim was to develop ideas, implement experiments and see results on a super-fast time scale. The groups were made up of biochemists, cell biologists, engineers, genomicists, theoretical chemists and physicists.

"The work we are doing is truly multidisciplinary, so being together at MBL has helped enormously in just finding the language we need to communicate, to understand how we are each are looking at the problem," says Rosana Collepardo-Guevara, who divides her time as a Professor of Computational and Molecular Biophysics between this department and the Department of Genetics.

"It was a bit different to most collaborations," comments Julia



Members of the Chromatin Consortium at Woods Hole.

Maristany, a third year PhD student in the Collepardo lab. "We had the same focus but in different fields: to see if experts on *in vitro, in vivo* and *in silico* could tackle a single biological question with different techniques. These were ambitious experiments: we brainstormed everything we could think of and took the most viable ones further. We'll be back next year!"

Thanks to the dedicated preparation beforehand, and diverse expertise, Rosana says the consortium members began half a dozen new research projects.

"We aim to establish a concerted effort across multiple laboratories and disciplines to advance the understanding of chromatin organisation via liquid-liquid phase separation."

Liquid–liquid phase separation looks at how two different liquids can remain distinct instead of forming a soup, like oil droplets suspended on water.

Transformative experiments in the past decade have shown that chromatin and its associated biomolecules can undergo liquid–liquid phase separation *in vitro* and in cells, forming liquid drops of differing chemical compositions–termed biomolecular condensates. Segregating different DNA regions, i.e. different genes, inside different biomolecular condensates is hypothesised to contribute to the tight regulation of gene function in the nucleus.

Continuing at Cambridge

Now that the groups are all back at their home institutions, the Collepardo group is using computer simulations to explore chromatin structure, and how it relates to gene regulation. They do this by developing powerful multiscale computational methods that can increase the resolution of experiments to near-atomistic levels, while at the same time revealing the physicochemical mechanisms that explain the experimental observations. These computer models need experimental data to complement their findings, which is where the work from the consortium comes in. The Collepardo lab's computational models uncover the molecular mechanisms explaining laboratory experiments and help design new experiments and, in return, the results of the experiments help the theoreticians refine their models and build new ones.

Julia adds: "Working in the same room was so important because we could talk in real time about the assumptions that we are making and bridge gaps in our understanding. We worked very well in the room together with everyone there for kick starting ideas.

"We're hoping to get some of the results out by the next consortium so that when we meet again the group can start on new ideas."

These in-depth studies of chromatins should advance the understanding of them across many fields and accelerate their role in medicinal research.

Dr Jan Huertas (left) and Maria Julia Maristany at the consortium

Quantum friction

It has been one year since Dr Stephen Cox became a Royal Society University Research Fellow. Since then, he and his growing team have been busy figuring out the fundamentals of friction between individual atoms.

Friction plays a role in our day-to-day lives, such as rubbing your hands together to generate heat on a cold day. Stephen's group looks at friction on a much smaller scale. They specialise in using computational techniques to test the validity of theoretical ideas in chemistry: especially in describing the friction of liquid water flowing over carbon surfaces at the atomic level.

These calculations are the foundation of research into emerging technologies. They inform what direction laboratories should take when studying water flow on carbon surfaces.

"What we do is the basis for a lot of emerging technologies in fields like desalination and generating renewable energy," explains Stephen.

PhD student Anna Bui adds: "By understanding the mechanism governing water flow at this scale, we can provide a molecular control of the flow by careful design of filtration membranes and nanofluidic devices, offering sustainable solutions to problems in water desalination and blue energy harvesting. For example, strategies to lower the friction can increase the efficiency of energy transfer."

Dr Stephen Cox.

Anna Bui.

Curious forces

The group has been using computational methods to test new, ambitious theories about what precise forces are at play at the atomic level. Anna's latest paper explores the idea of quantum friction to explain the forces between individual atoms. Quantum friction is a theory that predicts how quantum forces affect the motion between two particles[1].

Anna tested this new theory using computational techniques and found evidence that generally supports quantum friction.

"We can see that something like quantum physics is a good candidate for explaining these molecular interactions," says Anna. "If we can understand the forces from a molecular point of view then that gives more credit to the theory, and helps scientists down the line to turn these ideas into more practical applications."

Graphite, graphene, and everything between

The group is also investigating the flow of water over carbon-based materials, like graphite and graphene. These two materials have very different structures and a variety of properties. Graphite is soft and layers slough off, which makes it a good material for pencils. But graphene has a high strength thanks to the strong covalent bonds between the carbon atoms. Water behaves quite differently with these different surfaces.

"Intuitively we think: the rougher the surface is, the higher the friction is, but for these carbon surfaces that idea doesn't explain all the details," says Stephen. For example, graphene is a thin, strong sheet of carbon atoms that can be rolled into tubes thinner than a strand of hair. This research will help other scientists whose research involves water flowing through tubes, which has potential applications in energy storage, medicine and chemical sensing. The Cox group is paving the way for these new discoveries.

[1]Bui AT, Thiemann FL, Michaelides A, Cox SJ, *Classical Quantum Friction at Water-Carbon Interfaces, Nano Lett* (2023) 23, 2, 580-587.

Producing clean water and fuel from the sun

Researchers in the Reisner group have developed a floating device that can transform sunlight into purified water and sustainable fuel.

Artificial leaf hitching a ride on a punt.

From left: Chanon and Ariffin in the field.

Reisner group members Dr Chanon Pornrungroj and Ariffin Mohamad Annuar have created a way to produce solar fuels and purify water in the same device. The device not only works with contaminated water and seawater, but also does not require outside power, giving it far-reaching potential for remote or developing regions.

Artificial leaves

The device is called an 'artificial leaf' because it takes its inspiration from photosynthesis, the process by which plants convert sunlight into food. The group's earlier artificial leaves could produce green hydrogen fuel from clean water sources, but this new 'leaf' goes one step farther by producing both fuel and purified water at the same time. It even produced clean water from the River Cam in central Cambridge–quite a feat as anyone who is familiar with the river will attest!

Tricky

"Bringing together solar fuels production and water purification in a single device is tricky," says Chanon, who has recently returned to Thailand to take up a faculty position to develop sustainable technologies. "Solar-driven water splitting, where water molecules are broken down into hydrogen and oxygen, usually needs to start with totally pure water because any contaminants can poison the catalyst or cause unwanted chemical side-reactions."

"In remote or developing regions, where clean water is relatively scarce and the infrastructure necessary for water purification is not readily available, water splitting is extremely difficult," adds Ariffin, a second-year PhD student in the group.

"A device that works using contaminated water could solve two problems at once: it could split water to make clean fuel, and it could make clean drinking water."

Floating photocatalyst

To make the device, Chanon and Ariffin deposited a photocatalyst on a nanostructured carbon mesh that is a good absorber of both light and heat, generating the water vapour used by the photocatalyst to create hydrogen. The porous carbon mesh helps the photocatalyst float and keeps it from the water, so the contaminants can't reach it.

Potential benefits

A device that can make clean fuel and clean water at once using solar power alone could help address the energy and the water crises facing so many parts of the world.

"It's such a simple design as well: in just a few steps, we can build a device that works well on water from a wide variety of sources," says Chanon.

Professor Brian Thrush 1928 – 2023

Professor of Physical Chemistry Brian Thrush, who died on 14 September, brought together the separate Chemistry Departments in the 1980s as the first Head of a united Department of Chemistry.

Many alumni will remember that although both departments moved to the new Lensfield Road building in the late 1950s, they remained scrupulously segregated. Ronald Norrish led Physical Chemistry from the North side of the building and Alexander Todd presided over Organic and Inorganic Chemistry on the South side.

Brian himself recounted that in the 1950s there had been a proposal to join the two departments, but the strong factions involved (along with the famously slow-turning wheels of university administration!) meant that almost 30 years passed before this happened.

Early days

Brian came up to Emmanuel College in 1946, first as a Natural Sciences undergraduate and then as a PhD student in the Department of Physical Chemistry. Brian started his research under Morris Sugden but was quickly "pinched" by Ronald Norrish because of his expertise in electronics. Brian helped Norrish and George Porter (later Lord Porter) develop their flash photolysis apparatus for the study of extremely fast chemical reactions, for which Norrish and Porter later won a Nobel Prize [See Chem@Cam Winter 2017].

Research

After a sabbatical in the US, Brian returned to Cambridge and continued to investigate free radicals, chemiluminescence, kinetics and spectroscopy.

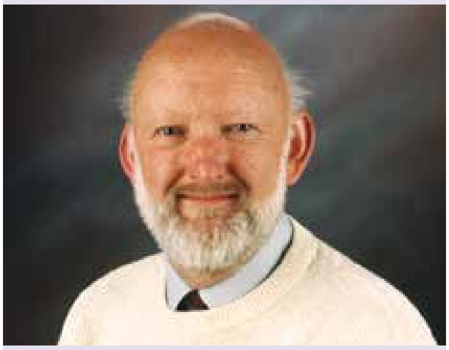
Amongst his many other achievements, Brian developed a new method of studying hydrogen atom reactions, and determined the rate constants of a series of nitrogen, hydrogen and oxygen atom reactions important in combustion and in the upper atmosphere. Brian won the Royal Society of Chemistry Tilden Prize in 1965 and was elected a Fellow of the Royal Society in 1976.

Brian's research areas were central to the developing science of atmospheric chemistry, which had previously not been considered a separate field of research. As a Natural Environment Research Council member, Brian promoted the development of New Blood lectureships, which helped to establish atmospheric science as a core field.

Wine

Brian was also acting master at Emmanuel College for a time and the Wine Steward for many years – in addition to his many other talents, he was always good to go to for advice about wine!

Dr Malcolm Gerloch 1939-2023



Malcolm Gerloch, who died on 24 September, came to the department from UCL in 1970, when Jack Lewis joined as the Professor of Inorganic Chemistry. Malcolm's research focused on the development of theoretical models to understand the electronic and magnetic properties of transition metal compounds.

Malcolm retired in 1999 to Canberra, Australia, where he lived with his second wife, Gwyneth. In retirement Malcolm wrote some dozen children's books and a collection of short stories, to add to his four technical books and over 120 research papers.

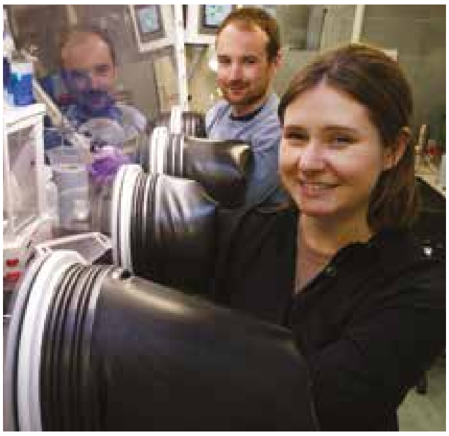
Noticeboard

Honorary doctorate for alumnus

Kelly Chibale (Queens' 1989) has been awarded an Honorary Doctorate by the University of Basel for his exceptional and inspiring curriculum vitae, his outstanding academic achievements, and his ongoing support of the Swiss Tropical Public Health Institute. Read more about Kelly on page 16.

Emerging Tech award for spinout

Wright group spinout Lambda Energy, which manufactures nanomaterials for greenhouse windows to turn harmful UV light into more wavelength friendly light for growing plants, has won in the category of Passive Light Management for Greenhouse Horticulture in the RSC Emerging Tech competition.



Outreach award for Grey group

Research Assistant Megan Penrod from the Grey group was awarded the Faraday Institution Community Award in STEM Outreach for engaging and inspiring young people in science. Alongside her research on lithium nickel oxides, Megan has been running STEM workshops in schools.

Macmillan Coffee Morning

In September, bakers from across the department poured sugar, flour and love into their homemade bakes to support the annual Macmillan Coffee Morning. The wide selection of goods on offer this year not only tempted our sweet tooth, but also raised £435 for support for people living with cancer.

Reisner group comes Full Circle

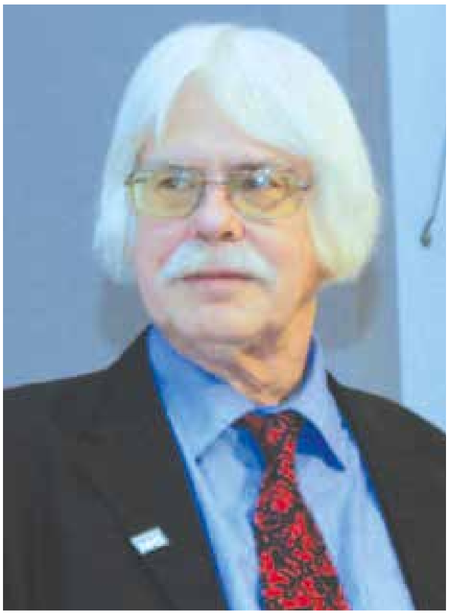
Professor Erwin Reisner and his group hosted an entertaining and instructive talk for the Alumni Festival. The team demonstrated their research-based solutions to climate change, waste and pollution, and showed how their work contributes to a sustainable, circular economy.

Student captains Uni Challenge team

First-year PhD student Ryan Kang is captaining the Trinity College University Challenge Team, which had a convincing win over Warwick in the second round after beating Southampton in the high scoring losers play-offs. Who knows how far they will go?

Letter to the Editor

We always love to hear from our readers, please tell us what you think!



Dr David Bullock at his retirement celebration, 2017.

From David G Bullock (Churchill 1969)

It was most pleasing to read about Choonzo Chiyumba's work on metalloenzymes (Chem@Cam Issue 66, Spring 2023).

I worked on organometallic catalysts (cobalt carbonyl) at ICI in Billingham between school and Churchill, and had supervisions with Stuart Warren. I have had the privilege to visit Zimbabwe twice (including a crossing into Zambia at Vic Falls) in my subsequent career in Clinical Chemistry.

With best wishes,

Dr D G Bullock
(Churchill 1969)

Editor's note: David writes that since leaving the department, he moved into clinical chemistry and worked at the Wolfson Research Laboratories in Birmingham. In 1979 he specialised in external quality assessment (EQA) and completed an in-service PhD in 1987, which he says "stretched the university's regulations on length – probably beyond the limit!"

For many years until his retirement in 2016, David directed Birmingham Quality, the main chemistry centre for the UK National EQA Service. He was founding Chairman and first President of the UK NEQAS Charity, and was recently honoured with the RSC L. S. Theobald Award, which is made to someone who has made a significant contribution to the development of analytical chemistry.

Tell us what you think

Do you like the crossword? Do you want to read more articles about staff, or find out what other alumni are doing? Are our articles too scientific or not scientific enough? Please take our survey to help us improve Chem@Cam for you, our readers.

You can email your response to news@ch.cam.ac.uk or post to Chem@Cam, Yusuf Hamied Department of Chemistry, Lensfield Road, Cambridge, CB2 1EW.

1. What do you like best about Chem@Cam?

2. What stories would you like to read in future Chem@Cams?

3. How could Chem@Cam be improved?

4. Do you prefer the printed or email version or both?

5. We would appreciate any further comments:

Seasonal Chemistry Cryptic Crossword

Challenge yourself with a cryptic crossword designed by Dr Mary Wood, a postdoc in the Zhang group, who researches electron transport.

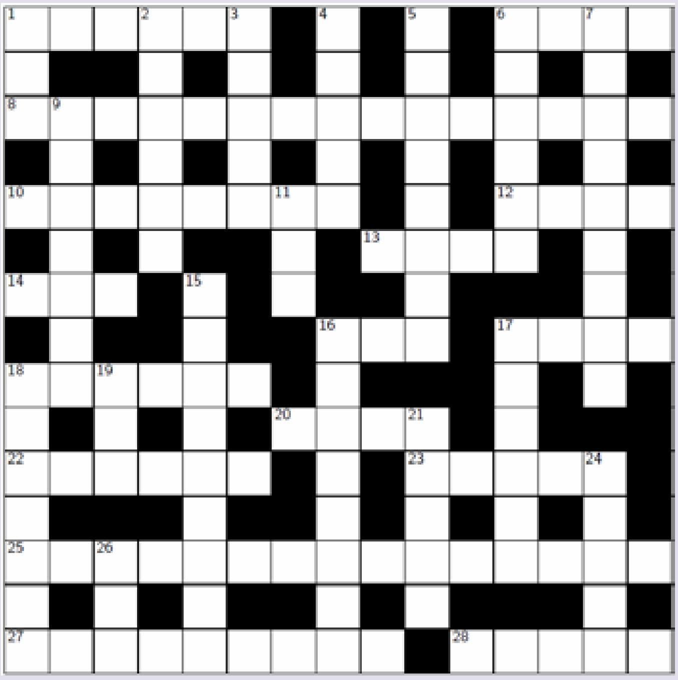
Mary is preparing for a new post at the University of Copenhagen where she will be investigating artificial photosynthesis. Thank you so much for the world-class crosswords, Mary, and we wish you the best of luck in your new post! Additional thanks to Dr Becky Welbourn, an alumna who was part of the Clarke group.

Across

1. Sparkly frippery: titanium is not French salt. (6)
6. Professor with expertise in extracellular matrices is owed, right? (4)
8. DNA expert is a ban, a mural ban, muddled up. (15)
10. Dye slits mangled and made unrealistic. (8)
12. A lone, backwards molecule (4)
13. Sounds like 2 down without the oxen—wait, don't go! (4)
14. Morning phosphorus is very current. (3)
16. Sounds like star that arrived at Christmas. (3)
17. Teaching assistant has head of iron—rather cheesy. (4)
18. Catalyst sounds like many good massages. (6)
20. Fruit for a Christmas drink—misheard, it isn't nippy. (4)
22. Solvent containers found in road of woes. (6)
23. Politician on coach comes up with quirky rowing competition. (5)
25. Shiny aircraft? XIX has two. (10,5)
27. Party essential—prison guard from South-West Ireland? (9)
28. Vacuum flask sounds like 6 across. (5)

Down

1. Dagger thrust a non-starter, for a new web-page. (3)
2. Ancient maternity ward seems pretty sturdy (6)
3. "Sounds like the home of cricket!" she praises. (5)
4. Woman's optical density reveals grumpy king. (5)
5. Mr Simpson scores a century at Cambridge college. (8)
6. Clue following academic finds transport fit for a mother and her king. (6)
7. Most of chemistry workspace between two English—seems rather complicated. (9)
9. DNA sample in French sea following appropriate article. (7)
11. Endlessly level on the night before Christmas. (3)
15. See Mr Lamb confused, making chemical preservers. (9)
16. Sounds like comfort hides the road to extreme days. (8)
17. Pretentious supper revealed by extreme rhythm in baby horse. (6)
18. Phase's knightless stratagem of the stomach? (7)
19. E.g. joule, angstrom endlessly reveals abbreviated institution. (3)
21. English precedes French half-sweet and yttrium in dense material. (5)
24. Bug in South Africa? What a creepy old guy! (5)
26. Christmas tree found in reef iridescence. (3)



Win a prize

Send a photo of your answers by 31 December to crossword@ch.cam.ac.uk for a chance to win a sustainable Yusuf Hamied Department of Chemistry travel mug. The first correct answer to be drawn after the deadline will win.

Answers will be sent out in our January alumni email. If you don't receive our emails, please make sure you've opted into receiving emails by logging into the University of Cambridge alumni website (www.alumni.cam.ac.uk).

Save the dates

After a four-year break, Professor Peter Wothers will resume his popularly acclaimed and highly explosive demonstration lectures at our Chemistry Open Day on Saturday 16 March 2024.

We have secured 100 tickets exclusively for the use of alumni and their families (limit of four per family) to see Peter's 11am lecture, followed by a buffet lunch in the Unilever Lecture Theatre Foyer. You are, of course, welcome to come for the entire Open Day to take part in all the science activities and demos, from the infamous slime pond to molecule building and beyond!

To ensure your reservation, watch out for our alumni email in January with further details. Please note the Open Day and Peter's lectures are not suitable for children under age 8.

A symposium featuring a day of talks to mark the scientific contributions of Professor John Pyle, who has retired as the 1920 Professor of Physical Chemistry, will be held on Friday 12 April 2024, followed by a reception in the department and dinner at St Catharine's College. For further information or to register, please email john.pyle.symposium.2024@gmail.com.