



# UCL

## UCL Chemistry NEWSLETTER

### Introduction by Claire Carmalt Head of Department

When I wrote the welcome to last years newsletter I didn't imagine that we would still be coping with the challenges of the Covid-19 pandemic a year later. We have managed to keep the department open since June 2020 (partially initially and now fully open), largely due to the efforts of all in the research school who followed the new Covid safety rules brilliantly. It was good to see people back in the laboratories and experimental research taking place again and a huge thank you to Steve Price and Rob Wilson who were very effective at ensuring the safety guidelines were followed. The final year undergraduate and master's students were able to do their experimental projects and we hope that this will continue into next academic year. It was a tough academic year for both staff and students with many rapid alterations being required, coping with remote working, home schooling, lockdowns etc. So I want to thank all the staff and students for their hard work, patience, understanding and their efforts in maintaining a great community spirit.

We had a number of retirements this year including Liz Read (Departmental Manager), Brian Kavannah (Safety Officer) and Judith James (HR), all of whom had been with us for many years. Dr Jon Wilden, Frances Thomson, Thom Dixon and Dr Lorena Ruiz-Perez left the department to move to new roles. In professional services we welcomed Enrico Buonauro (Research), Monwara Seetul (PG Teaching & Learning), Holly Ambrose-Wilson (Teaching & Learning), Hayley Dansey (HR) and Daniel Underwood (Research) into our team. Ruth Wilkinson joined us as Departmental Manager and Yael Moscou moved role from Senior Research Administrator to Deputy Departmental Manager. Luka Nunar joined us as a lab technician.

This academic year we were pleased to welcome three new Associate Lecturers (Teaching) to the department - Dr River Riley, Dr JL Kiappes Jr and Dr Miguel Rivera - specialising in Student Experience, Chemical Biology and Computational, respectively. Dr Fabrizia Foglia was awarded an EPSRC fellowship.

We were delighted with the news that Professor Richard Catlow received a Knighthood in the 2020 Queen's birthday honours for services to leadership in science and research. Dr David Scanlon was awarded the Royal Society of Chemistry (RSC) Materials Chemistry Division Early Career Award and

Professor Vijay Chudasama the RSC Hickinbottom Award. Professor Matt Powner was honoured in the prestigious 2021 Bavatnik Awards in recognition of his work on the origin of life. Dr Vicky Hilbourne, a Lecturer (Teaching) in the department, received a UCL Provost Education Award for the contributions she has made to assessment and feedback. A pleasant surprise for myself was being nominated and winning a UCL One Leadership Award for Outstanding Contribution. We were also delighted that the Department was awarded an Athena Swan Silver Award, as well as the Chemistry Equality Diversity and Inclusion (EDI) Team being chosen as winners of the Departmental Award for EDI Excellence in the UCL Inclusion Awards.



The department had a record intake for 2020/21 with 238 undergraduate students joining the department. In response to the pandemic the department developed an integrated programme of practical activities that allowed the 1st year students to do all of their practical's at home and you can read more about how this went in this newsletter. This exciting initiative, led by Professor Andrea Sella, provided students with a box of instruments with the principle that "if you can measure one molecule you can measure them all". The team won a MAPS Faculty Education Award. Despite the remote working, a hugely impressive number and quality of publications have

been produced from departmental research in the past year. This year we have also managed to restructure the research divisions in the department developing five Research Themes: Chemical Sustainability; Chemistry and Light; Materials for the Future; Chemistry and the Environment; and Chemistry for Life to go beyond the organic/inorganic/physical chemistry boundaries. This more thematic structure provides the opportunity for enhanced collaborations and discussions.

I have been enjoying being back in the building more often and I am looking forward to seeing more colleagues and students as we transition back to being on campus. I wish you all the best for 2021/22 academic year.

Professor Claire Carmalt

# LAB14

Practical Science in  
a Pandemic World  
Special Feature  
Page 14

## Contents

Staff Highlights	2
EDI	6
Student Highlights	8
CPS Report	10
Lab 14 Special Feature	14
Research Highlights	26
Alumni	34
Publications	38
Grants	50
Staff	51

## Acknowledgments

Editor:  
Prof. Claire Carmalt  
Editor at large:  
Dr Rebecca Ingle  
Design:  
Louise McSeveny

Heartfelt thanks to all our staff and student contributors, your efforts are much appreciated.

If you have an item for next year's newsletter we would love to hear from you. Please email [l.mcseveny@ucl.ac.uk](mailto:l.mcseveny@ucl.ac.uk)

# Staff Highlights & News

## New Appointments

### Dr Miguel Rivera



Miguel Rivera was born to Colombian parents in Strasburg, France. He moved to the UK to study Physics at UCL, after which, he carried out a PhD at Queen Mary University of London in computational method development for photochemistry in molecular crystals with Dr Rachel Crespo-Otero. During this time, he developed the FRamewOrk for Molecular AGgregate Excitations (fromage), a Python package which features QM/QM<sup>2</sup> geometry optimisation, conical intersection search, exciton analysis, and geometry manipulation of molecular aggregates.

He then became a postdoctoral researcher at Imperial College London where he studied polaron transport and ferroelectricity with Prof Aron Walsh, and contributed to the Julia code CarrierCapture. He joined UCL in February 2021 as an Associate Lecturer (Teaching) in Computational Chemistry.

Miguel has expertise in programming and electronic structure techniques, and is committed to democratising these disciplines by engaging with the Free Open Source Software community. He is dedicated to spreading his enthusiasm for getting computers to calculate wavefunctions. He is particularly interested in developing visualisation techniques to unlock better intuition of fundamental topics of Computational Chemistry.

In his free time, he plays jazz guitar, cooks, and plays many games from Chess to Dungeons & Dragons.

### Dr River Riley



River Riley is an Associate Lecturer (Teaching) with a particular focus on student experience. His role encompasses many aspects of student life within the department, including academic development, pastoral support, outreach and public engagement. Over the years he has worked to promote equality, inclusion and diversity initiatives and continues to embed these principles in his work in the department, particularly within his role as LGBTQ+ Champion.

River completed his undergraduate in chemistry at UCL in 2014 before continuing onto PhD research in spectroscopy with Professor Helen Fielding. During this time, he contributed to the design, construction and commissioning of the UK's first liquid-microjet photoelectron spectrometer. He later took up the position of Research Associate and Teaching Fellow in Physical Chemistry at UCL for two years, in which he lectured on the subject of molecular spectroscopy and laser chemistry. River's research interests remain in this field, but are now more centred around pedagogical approaches to spectroscopy and instrumentation.

### Dr J. L. Kiappes



J. L. Kiappes joined the department in February 2021. Born in Houston, Texas, USA, he earned his first degree from Rice University, before doctoral studies as a Skaggs–Oxford Scholar in a joint programme between The Scripps Research Institute (La Jolla, California) and the University of Oxford. At Scripps, he pursued the total synthesis of the natural product shishijimicin A in the research group of Professor K. C. Nicolaou.

Upon moving to the UK, J. L. joined the group of Professor Nicole Zitzmann in the Oxford Glycobiology Institute, where his focus shifted to medicinal chemistry and the development of novel antiviral therapies.

After finishing his DPhil, J. L. remained in Oxford as the Lerner–Fink Fellow in Medicinal Chemistry in the Department of Biochemistry and took up a Lectureship in Organic Chemistry and Biochemistry at Corpus Christi College.

As well as continuing to work on antiviral small molecules, his work expanded to include studies of other glycan processing enzymes, using biophysical methods and organic synthesis to develop medicinal candidates and chemical biology tools. During this time, he had the opportunity to contribute to lecture, practical, and tutorial teaching.

With this passion for teaching, J. L. was thrilled to join the Department as an Associate Lecturer (Teaching), contributing to organic chemistry, chemical biology and more generally chemistry at the interface with biological sciences. He is excited to collaborate with colleagues in the Department to develop innovative ways to support student learning and success.

### Dr James Attwater Royal Society University Research Fellow



James completed his PhD research at the MRC LMB in 2011, studying the activities of synthetic RNA catalysts in altered reaction environments as models of early life forms. During a Junior Research Fellowship at Homerton College and in subsequent postdoctoral studies at the LMB, he explored RNA interactions with vesicles, peptides and substrates, and developed an RNA catalyst capable of self-synthesis.

Beginning his Royal Society URF in 2021, he will investigate the origins of protein synthesis.

## Promotions

We are very proud to announce the following senior promotions of the department, effective from 1 October.



Jamie Baker to  
Professor in Organic Chemistry



Stephen Potts to  
Associate Professor (Teaching)



Gemma-Louise Davies to  
Associate Professor in  
Materials Chemistry

## Blavatnik Awards

### Prof. Matthew Powner



Professor Matthew Powner is one of nine UK recipients of the 2021 Blavatnik Awards for Young Scientists in recognition of his work on one of the world's greatest mysteries – the origin of life.

The awards, issued by the Blavatnik Family Foundation and the New York Academy of Sciences, are open to scientists aged 42 or younger. They aim

to recognise research that is already transforming technology and our understanding of the world.

Professor Powner, one of three young scientists honoured in the Chemistry category, was recognised for developing a “systems chemistry” approach to the origin of life – that is, studying properties that emerge in networks of molecules and cannot be attributed to individual molecules in isolation. This has led to a better picture of how chemical reactions could underpin the formation of life on the early Earth.



# RSC Awards

## Prof. Vijay Chudasama



Prof. Vijay Chudasama has been awarded the Royal Society of Chemistry's Hickinbottom Award for 2021 for the development of reagents and strategies for site-selective protein modification to enable targeted therapy, imaging and diagnostics.

Vijay is a Co-Founder/Director of UCL spin-out ThioLogics™. He has won multiple prizes and awards (departmental, faculty,

national, international) throughout his academic career such as the UCL Faculty of Mathematical and Physical Sciences Medal (2008), UK Science, Engineering and Technology Chemist of the Year (2008) and the Ramsay Medal (2011).

Vijay's research lab works in a variety of fields but one of the main focuses has been on providing site-selectively modified protein and protein-nanoparticle conjugates to enable targeted therapy and imaging. The protein element (usually) selectively targets a biomarker that is overexpressed on cancer cells (as compared to non-cancerous cells) and the nanoparticle or cargo that is appended to said protein provides tumour cell killing or imaging properties or both for applications in therapy, imaging and theranostics (respectively).

Vijay has research interests in the development and application of novel methodologies in Organic Chemistry/Chemical Biology, resulting in over 85 publications and patents, including highlights in Nature Chemistry, Nature Chemical Biology, Nature Communications, Nature Reviews Chemistry, PNAS USA, ACS Nano and Chemical Science.

## Prof. David Scanlon



Prof. David Scanlon has been awarded the Royal Society's of Chemistry's 2021 Materials Chemistry Division Early Career Award.

David is Chair of Computational Materials Design where he leads the Scanlon Materials Theory Group (SMTG). The group's work is at the forefront of the global effort to explore new materials based on computations and to advance the capacity of

first-principles calculations to predict materials properties. The group is currently working on new materials for Li-ion batteries, understanding novel materials for photovoltaics and photocatalysis, and optimising materials for thin film displays.

The SMTG uses computational models to understand what actually happens on the atomistic scale in materials that are of interest for many applications in renewable energy. We also use these models, which are based on computational chemistry, to predict new materials, or to predict the property of materials. These insights will allow for the design of better materials that we use in our everyday life. For example, we work on understanding the materials that are used in the screens of smart phones, tablets, laptops, flat screen TVs etc. The knowledge we gain on how these materials actually work on the atomic scale, can be used to tweak their properties, and inform experimentalists so that better materials can be developed, improving the quality of our device performance.

The group regularly publishes with experimental groups working in complementary areas of materials science from around the globe.

# Provost Education Awards

## Dr Victoria Hilborne

Vicky is a Lecturer (Teaching) and is a recipient of one of this year's Provost Education Award. These awards recognise staff making outstanding contributions to the learning experience and success of our students.

Vicky joined UCL in 2016 and has worked to develop new teaching in analytical and physical chemistry with an interest in application to environmental chemistry. Vicky has substantially developed and modernised new physical and analytical chemistry laboratory classes, the focus being on research skill development.

By shifting a whole year's assessment to coursework and integrating formative and summative feedback within the Topics in Modern Chemistry courses, Vicky has taken a leading role which has impacted on the whole department and will continue to do so in years to come. Feedback from staff and students has been extremely positive about her contributions. To lead all these changes, alongside carrying out all her other teaching and administrative duties to an excellent standard, is really remarkable.



# UCL One Awards

## Prof. Claire Carmalt, UCL One Leadership Award for Outstanding Contribution

The UCL One Awards recognise, celebrate and reward our Professional Services and Academic colleagues who have demonstrated outstanding performance in their roles, contributing to the success of UCL.

Prof Claire Carmalt, has been awarded the UCL One Leadership Award for Outstanding Contribution. She led the Department throughout the pandemic in both an inspiring and reassuring manner, successfully embedding a business-as-usual attitude whilst allaying the many anxieties that this extraordinary time has presented to all of us. From the first days of the pandemic in the UK, Prof Carmalt has demonstrated the vision, commitment and inspiration that defines leadership and thus ensured that the Department of Chemistry would be one of the first to reopen in June 2020, becoming a template for other departments to follow. Her leadership throughout the pandemic has been outstanding.



## Nicola Phillips, Ways of Working: Personal Excellence Award

The Ways of Working: Personal Excellence Award recognises staff's commitment, outstanding service and integrity.

Nicola Phillips, Chemistry's Senior HR Staffing Officer, has consistently been innovative and proactive in devising best practice methods to support her role in providing an excellent HR service to staff and students. She has shown true commitment to promoting our values of equality, diversity and inclusion and founded UCL's Staff Disability Forum, which has now become the Enable Network. Nicola always looks for ways to support her colleagues and is passionate about empowering others. She is well-deserving of this award in recognition of her unstinting hard work and dedication.



# Faculty Education Awards

Each year the Faculty of Mathematical & Physical Sciences recognises excellence in teaching from staff through the Faculty Education Awards. We are delighted to be able to announce the Chemistry winners of the 2020 MAPS Faculty Education Awards.

**Teaching Awards: Excellence Anna Roffey** is an essential part of the postgraduate delivery team and has introduced innovative ideas to streamline assessments. She has been instrumental over the last year converting modules for remote delivery.

**Teaching Awards: Highly Commended Jamie Baker** has been foremost in the department's efforts, co-leading, with the Departmental Tutor, the rapid switch to remote teaching and online assessment.

**Support Staff Awards: Excellence Mike Kelly** has made an outstanding contribution, in particular with his work in the area of timetabling.

**Support Staff Awards: Excellence Joe Nolan** has also made excellent efforts during lockdown and re-opening of the department. Joe enabled the return of experimental PGR students, and ensured that all Covid-19 safety guidelines were implemented.

**PGTA Awards: Excellence Jasper Berry-Gair** has provided inspirational teaching throughout the challenging lockdown conditions.

**PGTA Awards: Excellence Ivan Clayson** has gone above and beyond in the excellent support he has provided, in particular in the development of video lectures to support students completing remote projects during lockdown.

**Team Awards: Excellence The Lab\_14 Team** has helped to enable 1st year students to do all of their practical work at home. See page 14.

**Team Award: Personal Tutoring Support In a Pandemic Dr Tamara Alhilfi, Dr River Riley, Ms Bikram Bains**

**The Chemical & Physical Society (CPS)** were recognised with a Faculty Education Award for their dedication and commitment. See page 10.



# Equality, Diversity & Inclusion (EDI) Committee Update

**Professor Claire Carmalt &  
Dr David Rowley**  
(Co-Chairs, EDI Committee)

## EDI Committee Update

Despite the continued remote working over the past year the EDI committee has continued to meet via MS Teams. Recently, we expanded the EDI committee with further targeted roles and welcoming undergraduate (Blake Parker) and Masters (Janis Romanopulos, Hunaida Bhabha) students as well as further staff. We already had an LGBTQ+ Champion (was Kristian Mears, now Dr River Riley) and a Wellbeing Champion (Tamara Alhifi). We have expanded to now also have a BAME Champion (Saf Mendez). Kristian and River have enabled an active LGBTQ+ network to be developed in the department.

We have also developed a new mentoring scheme, initiated by Nicola Philips, for Early Career Researchers and PhD students which aims at supporting, reflecting upon and steering the mentee's career and personal growth.

The EDI committee also developed surveys for staff and students to explore experiences and views on the department's working practices, particularly with all the necessary changes due to remote working.



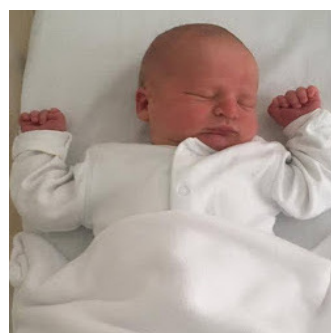
## Athena Swan Silver Award

Our Athena Swan Silver application was submitted in April 2020 despite being in lockdown at the time. We were delighted to learn in October 2020 that we have achieved a Silver Athena SWAN award in recognition of the impact the Department's actions and initiatives have made, and are making, on gender equality. The award reflects substantial effort from everyone in the Department to embed equality, diversity and inclusion in all our activities. This includes recruitment and promotion practices for staff and students, support for staff taking maternity leave, the promotion of female role models and the development of transparent workload models. We appreciate that the culture of valuing equality, diversity and inclusion improves the working environment for everyone. Professor Helen Fielding and Dr David Rowley led our submission with much support from the EDI committee and many other colleagues.



Chemistry EDI website:  
[www.ucl.ac.uk/chemistry/equality-diversity-inclusion-edi](http://www.ucl.ac.uk/chemistry/equality-diversity-inclusion-edi)

## Baby News



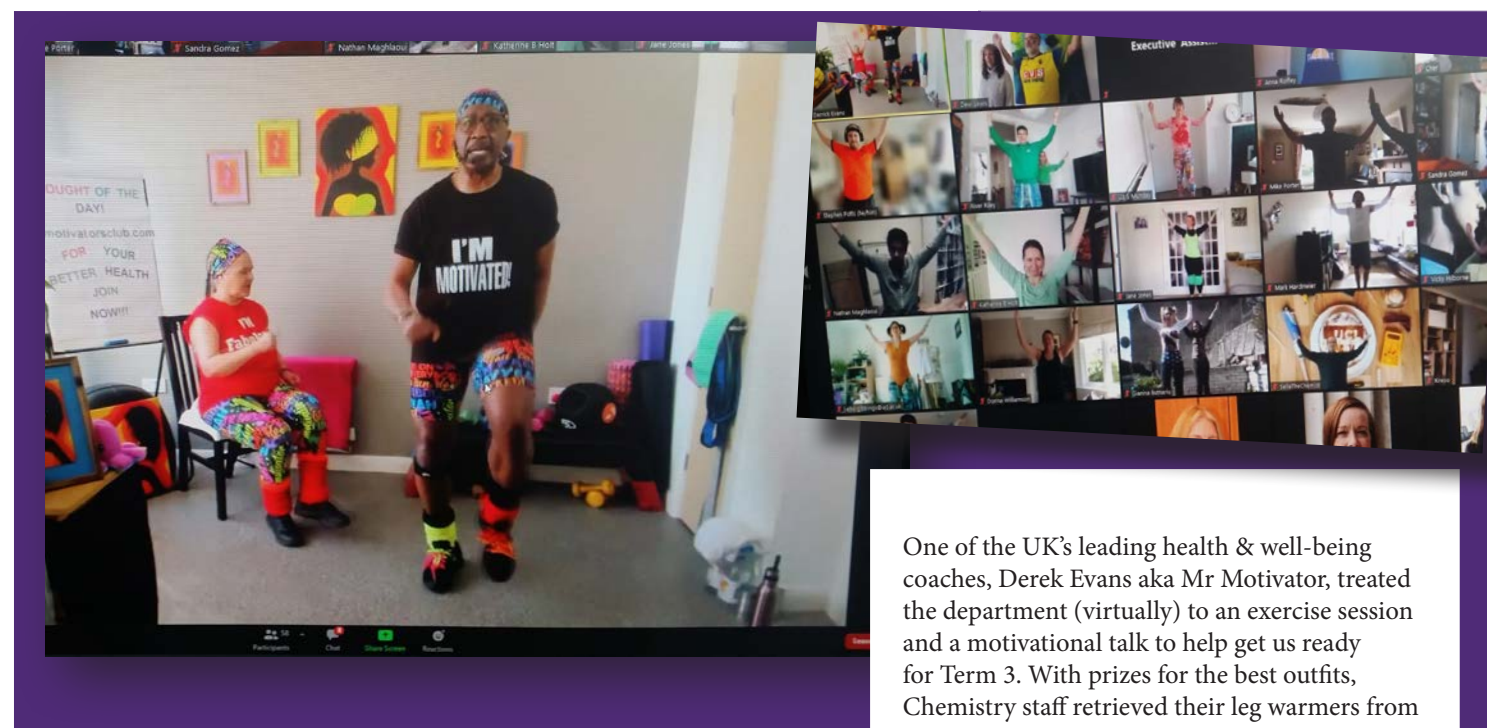
James Attwater and his partner Sarah had baby Jack on 06/05/21



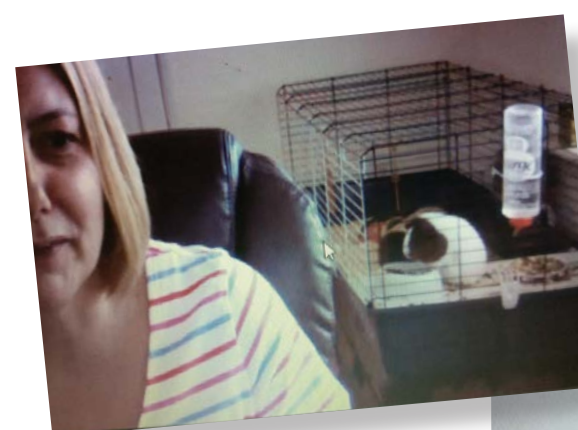
Sandra Gomez Rodriguez & her partner Clemens had baby Mateo on 13/12/20

## Departmental Award for EDI Excellence

Inclusion Awards recognise the work or contributions that individuals or teams make to progressing equality, diversity or inclusion practice within the institution. This department award is given to a UCL department or division that has demonstrated the most EDI commitment and impact over the past year. The department was thrilled to be chosen the winners of this award this year. It recognises the hard work and commitment that both past and present Chemistry EDI Team members have dedicated to EDI initiatives over the last few years.



One of the UK's leading health & well-being coaches, Derek Evans aka Mr Motivator, treated the department (virtually) to an exercise session and a motivational talk to help get us ready for Term 3. With prizes for the best outfits, Chemistry staff retrieved their leg warmers from the back of the cupboard and worked up a sweat, raising £500 for Mr M's charitable trust that supports various homeless charities throughout the UK. Thankfully there was an absence of lycra unitards.



Meet Chemistry Teams Meeting guests:  
Basil & Bertie (and Claire)  
Monkey (and Ruth)  
Herbert & Ness (and Yael)  
By popular demand Bertie & Basil get a close up





# Student Highlights & News

## 2020-2021 Prize Winners

### PhD Prize Winners

#### Ewing Prize

##### Joseph Broughton

Supervisor: Helen Fielding  
Best student presentation in Physical Chemistry for his presentation titled: Illuminating the Ultrafast Dynamics of Thiophene

#### Catlow Prize

##### Warda Rahim

Supervisor: David Scanlon  
Best student presentation in Computational Chemistry for her presentation titled Computationally Driven Discovery of Complex Oxide Materials for Thermoelectric Applications

#### Clark Prize

##### Katie Hobson

Supervisor: Claire Carmalt  
Best student presentation in Inorganic Chemistry for her presentation titled Aluminium Catalysed Alkyne Hydroboration: A Kinetic and Mechanistic Investigation

#### Davies Prize

##### Peter Aron Szijj

Supervisor: Vijay Chudasama  
Best student presentation in Organic Chemistry for his presentation titled Bispecific Antibodies and their Conjugates for the Treatment of Type 1 Diabetes and Cancer

### Second Year PhD Poster prizes

#### Inorganic Chemistry

##### Viliyana Lewis

Supervisor: Gemma-Louise Davies

#### Organic Chemistry

##### Alexia Rottensteiner

Supervisor: Stefan Howorka

#### Physical Chemistry

##### William Fortune

Supervisor: Helen Fielding & Katherine Holt

#### Computational Chemistry

##### Sean Kavanagh

Supervisor: David Scanlon

#### Rothwell Prize for Best Synthesis Work

##### Usman Shabbir

Supervisor: Tom Sheppard

## Roshni Malde Ramsay Medalist



Roshni Malde is the recipient of the 2020 Ramsay Medal.

Roshni graduated from the University of Birmingham in 2017 with an Msci degree in Natural Sciences. She then began her PhD studies at UCL under the supervision of Prof. Jamie Baker, Prof. Helen Fielding and Prof. Vijay Chudasama in the interdisciplinary fields of chemical biology and photochemistry.

Roshni's PhD research has focused on utilising ultrafast laser spectroscopy to study the excited states involved in novel photochemical reactions, deepening the knowledge of the photoreaction mechanisms.

These powerful photoreactions have then been applied to proteins and peptides towards the development of novel phototriggers and photocleavable conjugates for potential as therapeutics and probes.

Roshni is currently preparing manuscripts for publication and has presented her work at national and international conferences, most notably invited to give a talk at PEGS Europe 2019 in Lisbon.

Through her PhD, she has been awarded the Bader Prize, Physical Chemistry Poster Prize, Davies Prize and has now been awarded the Ramsay Medal. Roshni is now in the process of writing her thesis entitled 'The Study and Development of Photoactive Protein Bioconjugates' and aspires to continue her research career as a chemical biologist.

Roshni recently featured in the UCL MAPS podcast, Hypot-enthuse and answers the pressing question:

What is a Photoactive Protein Bioconjugate?

Listen here: <https://bit.ly/3o0xnFr>

### Graduating Students

#### Katya Ahmad

PhD

Supervisor: Peter Coveney

#### Alexander Aina

EngD

Supervisor: Sarah Price

#### Calise Bahou

PhD

Supervisor: Vijay Chudasama

#### Chia-Hao Chang

PhD

Supervisor: James Anderson

#### Katherine Chio

PhD

Supervisor: Tung Chun Lee

#### Benjamin Colville

PhD

Supervisor: Matthew Powner

#### Lewis Cowen

PhD

Supervisor: Bob Schroeder

#### Ioannis Galdadas

PhD

Supervisor: Francesco Gervasio

#### Alexander Gheorghiu

PhD

Supervisor: Peter Coveney

#### Alexandra Groves

PhD

Supervisor: Jawwad Darr

#### Alice Henley

PhD

Supervisor: Helen Fielding

#### Jennifer Herbert

EngD

Supervisor: Andrew Beale

#### Qing Hou

PhD

Supervisor: Richard Catlow

#### Faiza Javaid

PhD

Supervisor: Alethea Tabor

#### Jianwei Li

PhD

Supervisor: Ivan Parkin

#### Zilu Liu

PhD

Supervisor: Bob Schroeder

#### Kristian Mears

PhD

Supervisor: Claire Carmalt

#### Rushita Mehta

PhD

Supervisor: Robert Bell

#### Tina Miao

EngD

Supervisor: Tang Junwang

#### Caroline Nowicka-Dylag

PhD

Tracey Clarke

#### Anand Patel

PhD

Supervisor: James Anderson

#### Jordan Shaikh

PhD

Supervisor: Tracey Clarke

#### Zainab Sharif

PhD

Supervisor: Christoph Salzmann

#### Archie Wall

PhD

Supervisor: Helen Hailes

#### Yu Wang

PhD

Supervisor: Helen Hailes

#### Oscar Williams

PhD

Supervisor: Geoff Thornton

#### Jianxiong Zhao

PhD

Supervisor: Helen Hailes

### Undergraduate Prize Winners

#### Ouran Xie

##### Lysandre Rolland

##### Rozana Mazlumian

##### Nour Akhrass

##### Jingxuan Song

##### Lauren Cook

##### Kristina Kostadinova

All received the CK Ingold Prize for excellence in undergraduate performance.

#### Elizabeth Cosgrove

Ronald Nyholm prize for excellence Inorganic Chemistry

#### Cliona McMahon

Parke Davis prize for excellence in Medicinal Chemistry

#### Sadia Begum

Harry Poole prize for excellence in Physical Chemistry

#### Helen Spong

Neil Sharp prize for excellence in Theoretical (including Computational) chemistry

#### Francesca Ridgeway Bishop

Franz Sondheimer prize for excellence in Organic Chemistry

#### Aiman Bin Johanuddin

Charles Vernon prize for excellence in Biological Chemistry



The UCL Chemical and Physical Society (CPS) was founded in 1876 and is believed to be among the oldest, if not the oldest scientific student-staff body in the country. It is principally managed by students and hosts weekly academic lectures throughout term time, along with a plethora of social events throughout the year. The students are supported by academic staff who act as Presidents and Vice-Presidents in a mentoring and advisory capacity. Throughout this year, Drs Tamara Alhilfi and Krešo Bučar were pleased and eager to be on our side. Our lecture programme has a general science remit, while our audience is mainly comprised of staff and students of the Department of Chemistry and the Natural Sciences department, as well as the members of SCI London Group, who sponsor the Society. All our lectures are also open to keen members of the public. This makes the Society a wonderful place to connect with friends and colleagues over a cup of tea or a beer, while also talking about a little bit of science (or not!).

The pandemic imposed numerous challenges to the pursuit of our usual activities, and it marked the 145<sup>th</sup> anniversary of the Society with a big change – we went virtual and Zoom-ed it all! The Committee adjusted swiftly and sailed through this enormous transition smoothly, setting up several new online platforms. We hope that our new Moodle page (<https://bit.ly/3ihbVs3>), Eventbrite tickets portal (<https://bit.ly/3DenNn5>) and YouTube channel (<https://bit.ly/3AVvmxT>) will help everyone to fully enjoy what the Society has to offer. Now one will never have to miss a talk as all of our lectures are recorded and made available through the new platforms.

This year, we were also fortunate enough to become affiliated with Gradcracker (<https://bit.ly/3oh1rgl>), a careers website that showcases opportunities for STEM students and provides useful resources to those who are at different stages in their careers. Not only is this an important means for our undergraduate students, but also an opportunity for postgraduates who hope to explore opportunities for their career progression. We are very grateful to Miranda Molloy, our 2020-2021 Co-Secretary, for leading these efforts!

Facilitating Freshers Events during the pandemic was an exciting challenge, organised by our fabulous Events Team. It all kicked off with a virtual version of our famous **Pub Crawl**, with fewer pints, but more games. Later in the week, we held two **“Get to Know” sessions**, one for undergraduates and one for postgraduates, where students mingled online and had a

chance to socialise with their new peers. We hope we managed to jump-start a friendship or two. A fortnight later, there was also a **Fresher’s Quiz** using the previous year’s Christmas quiz questions (why not – they were so good!?) to bring everyone together once again before we went into the full swing of the term.

The Society was honoured to host a variety of speakers with a diverse scientific background. Since our lectures were delivered online, we were able to invite scientists from all over the world and were no longer restricted to speakers that are only a train ride away – the silver linings of the pandemic! We were particularly excited to host speakers who were at different stages in their careers and were happy to discuss their scientific journeys. Another novel and thrilling part of the CPS calendar were the Lunchtime Talks on Wednesdays. These were introduced to improve accessibility to our activities, as we realised that evening talks were impossible to attend for many members of the Society and the public who have other responsibilities. The lunchtime series was a big hit: we will certainly continue with it next year. An account of the events we hosted throughout the year follows below.

The lecture series started off with our long-awaited presidential talk (postponed due to the pandemic) from Dr Anna Roffey titled **“Are Pigeons Smarter than Mathematicians?”**, an interactive workshop on how birds seem to be better at solving the Monty-Hall problem than humans are! We then heard from Dr Katherine Elvira (University of Victoria) with a talk titled **“Artificial Cells on a Chip for Drug Discovery”**, who gave us a comprehensive overview of her research using microfluidic devices as a tissue model for testing potential drugs – and also for brewing micro beer. Our next speaker was Dr Swen Hoelder (Institute of Cancer Research) with a talk titled **“Discovering a Phase 1 candidate for the treatment of triple negative breast cancer”**. He introduced us to a medicinal chemistry approach to the prediction of effective treatments to tackle new mutations of the cancer. In her talk title **“The Inbetweeners - Methods beyond Born-Type models in Photoelectron Holography”**, Abbie Bray, (PhD candidate, UCL) discussed quantum interference in strong field laser-matter interactions and attosecond physics, as well as touching on the topic of gender inequality in STEM.

We then moved on to **“Diamond - more than a girl’s best friend?”**, a talk from our very own Professor Katherine Holt, on the chemistry of diamonds and their very varied



Our Secretaries Chiara Argenti and Miranda Molloy keeping safe with CPS face masks, taking a stroll in the park in February 2021.

In-person post-lockdown get together in March 2021. From left to right – Rachael Doherty, Sarah Wills, Blake Parker, Miranda Molloy, Krešo Bučar, Chiara Argenti.

Lovely June picnic with both old and new committee members. From left to right – Deepali Desai, Luca Petrini, Jakub Chomiuk, Lauryna Soblyte, Miranda Molloy, Lauren Cook, Hannah Thatcher, Blake Parker, Chiara Argenti, Sofia Rogers Ruiz.



uses. The next talk in the lecture series, presented by Dr Tommy Thompson (Kings College London), was titled **“Artificial Intelligence in Video Games: Past, Present and Future”**. He detailed the psychology behind his research into computer science, in a presentation inspired by the stylings of video graphics. Professor Jonathan Nitschke (University of Cambridge) continued the series and wowed us with his talk **“Incarceration changes behaviour, for molecules too”**. The presentation was all about metallo-supramolecular coordination cages and their use to transport cargoes of sensitive molecules.

In his talk titled **“Lapis lazuli – Medieval Materials Processing”**, Dr Spike Bucklow (University of Cambridge) outlined a process of mineral separation that was documented across Europe for over 1000 years that reliably created a blue colour for artists and a widely used drug. There was an unfortunate and unpleasant interruption from some ‘zoom raiders’ as he spoke, which was dealt with swiftly and professionally by the Committee. We have since updated our security settings! After the talk in our breakout room, we

had an interesting discussion on what authenticity means when it comes to antiquities, but also learned about his connection with the puppet show ‘Spitting Image’ and Jabba the Hut, a villain of the fictional Star Wars universe. In the final week of the first term, we heard from Professor Rachel Oliver (University of Cambridge) in her talk **“Illuminating Materials: the Materials Science of Light Emitting Diodes”**. She outlined her research on gallium nitride and how defects in the crystal structure affect the functioning of the semiconductor devices. The very last talk before the Christmas holidays, titled **“Sponges for Mitigating Environmental and Health Impacts of Polluted water”**, was delivered by Dr Pavani Cherukpally (Imperial College London) to emphasise the need for silicon nanoneedles as water purification devices. The first term was also full of other notable events. For example, we hosted several **“Speed Friending”** events during the first term. In this brand-new initiative, which was envisioned to help new students to connect, we gathered them into breakout rooms with one or two fellow undergraduate or postgraduate students. The students were ‘shuffled’ through many groups to ensure that everybody had chance to meet and

# Chemical & Physical Society

## Annual Report 2020-2021

by Chiara Argenti Co-Secretary

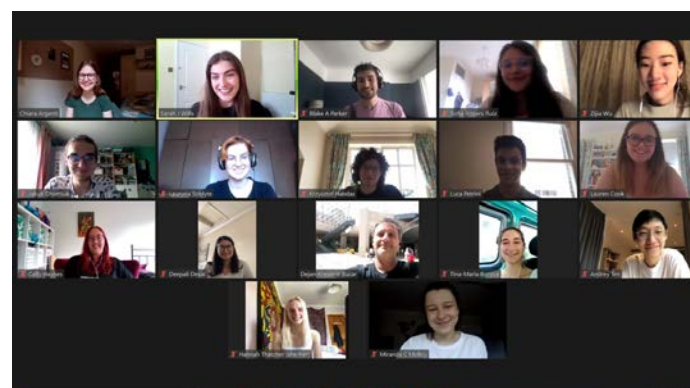




Screenshot of the presidential talk in March. On the right in the box highlighted – Tamara Alhilfi (CPS President 2020-2021). From left to right and top to bottom – Blake Parker, Sarah Wills, Krzysztof Habdas, Kristina Kostadinova, Chiara Argenti, Tina-Maria Burova, Miranda Molloy, Harry Li, Andrey Ten, Rachael Doherty.

We then had a very topical lecture from Dr Rohin Francis (UCL) titled “**Science Communication During a Pandemic: are we Part of the Problem?**”, which covered the spread of misinformation during the COVID-19 outbreak and how we, as scientists, can better communicate with the public and press. Our next speaker, Professor Sapun Parekh (The University of Texas at Austin), spoke on chemical microscopy and its uses for the medical field in his talk titled “**Visualising Molecular Structure and Function in Soft Matter Using Vibrational Microscopy**”. Also from the United States, Professor Jonathan Wilker (Purdue University) next presented his research ( “**Adhesives at the Beach: Characterisation, Synthetic Mimics and Applications of Marine Biological Materials**”), which takes inspiration from sea creatures to make synthetic nanocomposite sealants. We then heard from Andy Extnance (RSC Chemistry World) in his talk “**Writing Science into Peoples Brains**”, wherein he discussed how lies spread faster than the truth, when it comes to the media and science communication. During reading week, we hosted a **Games Night**, during which we relaxed over numerous games, including Among Us and Jackbox – we even got quite competitive!

Starting off the second half of term after a short break, Dr Alex Archibald (University of Cambridge) illustrated the effects of the pandemic on air pollution in his talk titled “**COVID-19 and its Impacts on the Atmosphere: A Glimpse into the Future**”. We were then privileged to host Professor Dawn Shaughnessy (Lawrence Livermore National Laboratory). In her talk titled “**Looking Past the Periodic Table: the Discovery and Chemistry of the Super-Heavy Elements**”, she spoke on her involvement in the discovery of 5 new elements (114-118) by pushing the boundaries of the periodic table, answered numerous questions about fundamental nuclear science. After the talk we also bonded over our joint love of orange post-it notes. Back to the topic of climate change, Dr Ella Gilbert (University of Reading, British Antarctic Survey) brought a healthy dose of optimism to the topic in her talk titled “**Reasons to be Cheerful: Climate Optimism for Troubled Times**”. Next Dr Andrew Steele (Science Writer) presented his new book, “**Ageless: the New Science of Getting Older Without Getting Old**” using a very slick green-screen setup. Rumours emerged that some members of staff in our Department were impressed, while others were intimidated by it!



August handover committee meeting with both old and new members. From left to right and top to bottom – Chiara Argenti, Sarah Wills, Blake Parker, Sofia Rogers Ruiz, (Wendy) Wu Zijia, Jakub Chomiuk, Lauryna Soblyte, Krzysztof Habdas, Luca Petrini, Lauren Cook, Cally Haynes, Deepali Desai, Dejan-Kresimir Bucar, Tina-Maria Burova, Andrey Ten, Hannah Thatcher, Miranda Molloy.

befriend lots of new chemists. The annual **Careers Event** was again well attended. Our speakers, who have graduated with a Chemistry degree and gone into various career paths, talked about their experiences in the workplace and professional journey. This year we heard from Liam Door (patent attorney), Michael Barrow (conducting postdoctoral research with the UK Regenerative Medicine Platform), Jaclyn Raeburn (Cambrex Pharmaceuticals) and Robert Woodward (Assistant Professor, University of Vienna).

Our annual **Christmas Quiz** was, as usual, a big success, with a record-breaking number of 19 teams participating. Attendees stayed in breakout rooms for hours after the quiz ended and the whole experience was really fun and refreshing! The winning team, ‘Chemicallyfragilesticexpialezoomshous’ (no typos here!) was not the only one with a funny and original name built on a chemistry pun. We introduced an award for the team with the best Zoom background to fit in with the online atmosphere. This team was in fact one which had a recycled Christmas tree made of cardboard boxes and decorated with sweet wrappers! The competition was tough, but this was not only visually pleasing but also sustainable! We thank Dr Dewi Lewis for his continued support of the Quiz – he was an outstanding co-host.

Professor Harry Anderson (University of Oxford) kicked off the second term with his talk “**The Creation of Molecular Nanostructures with Unusual Electronic and Optical Properties**”, which was focused on the design and preparation of nano-scaled electronic circuits using molecular wires. In the same week, the Society hosted another virtual **Pub Crawl**, in a COVID friendly environment - we even all had Zoom backgrounds of different UCL pubs! The lecture series then continued with a talk from Dr Harry Cliff (University of Cambridge), titled “**The Future of Particle Physics**”, which sparked a healthy debate in the comments section of the YouTube video after the lecture gained over 22k views. Our next talk was by Madina Wane (PhD candidate, Imperial College London) and was titled “**Two sides of the Same Fish: Developing Tools for Scientific and Social Questions**”. She discussed the importance of developing new systems to explore scientific concepts and social issues, using her research on respiratory immunology in zebrafish as an example. Following the theme of social change Dr Lilian Hunt (Wellcome Trust) gave an engaging presentation titled “**Equality, Diversity and Inclusion in Science and Health Research: Collective Achievements, Actions and Ambitions**”.



Another highlight in our lecture series was an evening with Professor Omar Yaghi (University of California, Berkeley), who presented his pioneering research on metal-organic frameworks in a talk titled “**Water Harvesting from Desert Air**”. We were not only impressed by the new applications of metal-organic frameworks his group is exploring, but also by how generous he was with his time. Professor Yaghi happily and patiently answered a large number of questions for nearly two hours after his talk. The following day, Charlotte Williams (University of Oxford) spoke on polymerisation kinetics, and other important factors when making sustainable plastics, in her talk titled “**Catalytic Activation of Renewable Resources to Make Plastic**”. In her captivating talk titled “**Recombinant Spider Silk as a Novel Antimicrobial Biomaterial Using Click Chemistry**”, Dr Jolanta Beinarnoviča, (PhD candidate, University of Nottingham), outlined her research of silk-based synthetic nanofibres and explained how the cannibalistic nature of spiders and the inability to farm them necessitates the development of new synthetic production methods for these materials. We next heard from Krystal Vasquez (PhD candidate, California Institute of Technology) in her talk “**Measuring Atmospheric Compounds as a Disabled Chemist**.” She spoke on her PhD research, as well as highlighting the difficulties faced by disabled students across higher education and the need for universal design in laboratories. Professor Květoslava Burda (AGH University of Science and Technology, Krakow) presented the effects of reactive oxygen species in the living cells, focusing on erythrocytes, and our bodies’ natural way of protection via endogenous and exogenous antioxidants. Her talk was titled “**To oxidize or protect against oxidation - that is the question.**” Our final talk of the academic year was the presidential lecture presented by Dr Tamara Alhilfi titled “**Does a Good Cook Make a Good Chemist?**”. She explored the link between food and chemistry and used this as a metaphor for her redevelopment of the fourth-year lab course. She presented the pedagogy associated with teaching students how to be good synthetic chemists, as well as how to ensure equity for all students as they progress through their education.

For the very last event of the academic year, we hosted a **Mental Health Workshop** run by Dr Zoë Ayres, an analytical scientist, and a prominent mental health advocate, driving for change. She runs the #100voices project, an essential platform for sharing the mental health journeys of hundreds of researchers to help destigmatise talking about academic



January virtual CPS Pub Crawl advertisement.

Talk advertisement banner for Professor Omar Yaghi's talk in March 2021.

mental health; which can be found on her website <https://www.zjayres.com/>. The workshop inspired Chiara Argenti, our Co-Secretary, to develop a CPS Moodle tab (<https://bit.ly/3ihbVs3>) that focuses on mental health in higher education, and to collate resources that are available to students, but are often hard to find. We are very grateful for Chiara's initiative and efforts, and hope that this Moodle resource will be of help to our student body. We will continue talking about this important topic in years to come and have plans for our next workshop already.

Unfortunately, it still was not possible to host our post-exams boat party, but we will have to make up for this with an extravagant one in the coming academic year! On average, our attendance was at 37 participants per talk across our talks in the first and second terms of last year. We found our attendance to be consistent and our peak was 121 attendees, which is no mean feat (especially during a pandemic)! Our plan for the upcoming talks is to continue with our successful online strategy as before. We will continue hosting talks on Zoom until we can finally meet you all in the Nyholm room again. Hopefully in the second term, as there are some very exciting speakers lined up!

Lastly, we were incredibly excited and honoured to be shortlisted for a UCL Provost Education Award, and to receive a MAPS Faculty Education Award. We are grateful to UCL and the Faculty of Mathematical and Physical Sciences for their support, and their recognition of our endeavours to not only facilitate learning, but also to foster a friendly atmosphere among students in the department and build a sense of community.

If you would like to learn more about the CPS and our events this year, please do visit our website (<http://cpsucl.com/>), Instagram ([https://www.instagram.com/cps\\_ucl/](https://www.instagram.com/cps_ucl/)), Twitter (<https://twitter.com/CPSUCL@CPSUCL>) and Facebook (<https://www.facebook.com/CPSUCL>). It has been a privilege to be part of such a thriving Society this year.



# LAB 14

## Practical Science in a Pandemic World

With 238 incoming undergraduates, social distancing restrictions and the uncertainties of the Covid pandemic, Chemistry staff, led by Professor Andrea Sella, set about creating a chemistry set for adults; practical science of measurement and exploration for our students to engage with from the safety of their own home.

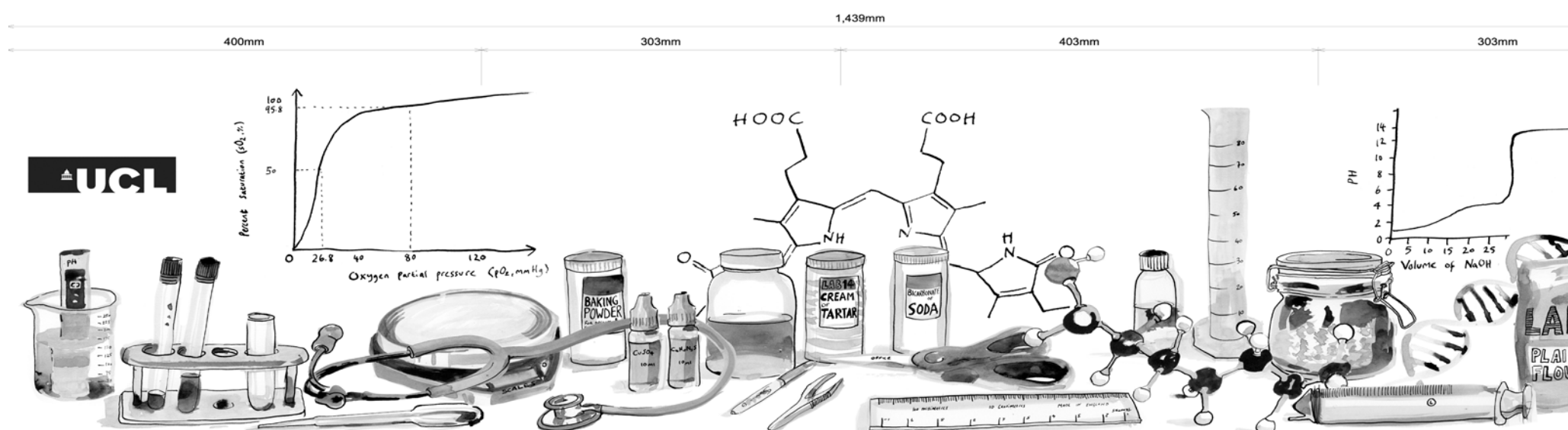
Lab 14 was rolled out beyond the Chemistry department, and students across the majority of Life Science courses at UCL experimented with these kits.

We caught up with Prof. Sella for a Q&A, and asked our Lab 14 students to describe the ups and downs of kitchen chemistry and offer top tips for the incoming class of '21.

Contributions & photos from: Andrea Sella, Natalia Sanchez Castro, Heike Munro, Sebastian Szkudelski, Winnie Sae-Seung, Michael Chan & Letizia Filippi

Additional photos: Helen Wong, Hannah Shalloe & 1st year undergraduates

Artwork: Ruby Wright



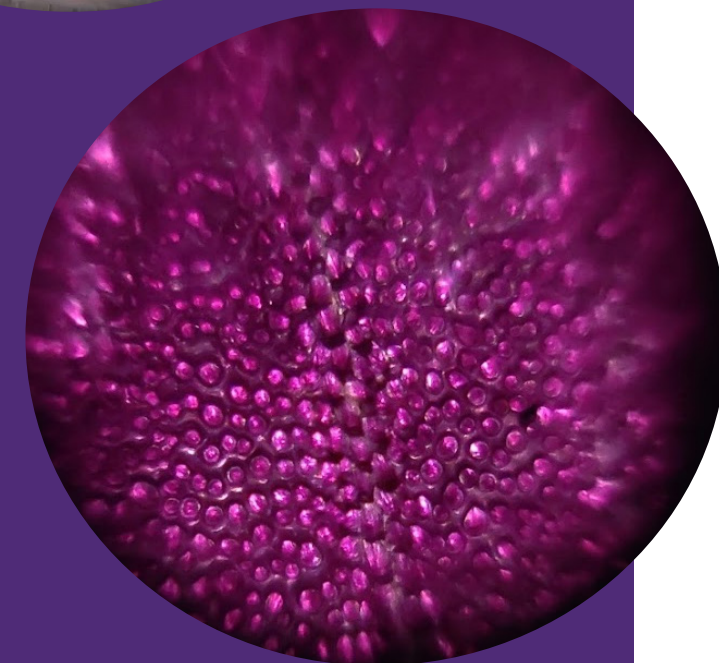




**“It is an  
adventure  
playground  
for grown  
ups”**



left: Box contents  
(Photo: Helena Wong)  
Right: top - bottom  
foldscope:  
moss  
pansy  
hair  
(photos Hannah Shalloe)



**Andrea: what is lab 14?** Lab 14 is the chemistry set updated for the 21st century. It is an adventure playground for grownups.

With the pandemic we found ourselves without the possibility of getting our students into traditional labs. Traditional chemistry sets for children were based on little bottles of some ‘stuff’ but sending ‘stuff’ through the post is not really possible, but the bigger flaw is that once you run out of ‘stuff’ you can’t do anything. So the idea we had was that instead of ‘stuff’ we send instruments.

Chemistry is not about chemicals it is about measuring them and studying them. If you send out a specific chemical you learn about that specific chemical. If you can measure one chemical, you can measure them all.

Instead of a closed practical with a narrow set of instructions, we would send a set of instructions for a set of activities where you could start with salt then try sugar or bicarbonate or cream of tartar. All these things you can find at home – it takes you to this idea of inquiry and improvisation. Many students get into a research lab and discover that the procedures they find in articles don’t work. The description on what you have to do is based on the writer’s perspective and is missing all kinds of imperceptible details. In the undergraduate labs we narrow down those descriptions so far that there is no room for error – it ensures that everyone can complete their work in the allocated time. It is not how the real-world works. In many ways we thought this was much more educational that would cover more ground with many more ideas.

There is a sense that if things don’t work in the lab then you are a failure – this is the wrong message. Learning constitutes failure – when we are trying to figure out how things work, we must have the time and pace to get things wrong.

There is the ritual of the lab – you put on a coat, your glasses, you sign in and you use this special equipment. In fact much of what we do can be done in pots and pans, one student can use a wine glass another can use a tea cup – it is still cream of tartar.

It is a very different approach from closed labs – 200 students given the same practical to write up – this was an opportunity for these conversations and a chance to be more creative.

**How did the idea start?** A brilliant ex UCL colleague Sarah Jane Blackmore at Cambridge sent me an email and asked for a list of chemistry related activities to do at home for her son who is interested in doing chemistry and wanted to prepare himself for university. I did not really have anything that was not totally trivial, there are primary school activities, but I would insult an A level student by telling him to make a baking soda volcano. For several weeks I did not reply as I was so upset that I did not have an answer. This triggered the thought of what is difference between the primary school activity and university? The fact is, it is exactly the same. Many of these activities emerged from a previous project called Lab 13.

**Which brings me onto the name. What is the significance of the name Lab 14?** The name Lab 14 is a joke. It is the year up from the lab 13 project, and going to university is year 14 of going to school. 14 refers to the dissociation constant of water where the equilibrium constant of water is  $10^{-14}$ . The  $pK_w$  of water is 14.

It was the thought that you could take a primary school activity but do it again to include measurement so that it is not just simply observational. If you have a pH meter then you can start to see a lot more of what the acid and the base are doing and that is where the intellectual side comes in – whether you do it with baking soda and vinegar or drain cleaner or kitchen descaler – the intellectual framework is the same. All you need is the instrument to record the data.

The whole thing was set up to reduce the pressure on students. We don’t have formal lab reports, it is not marked on whether you get it wrong – all you had to do is demonstrate you have done it. That will always come as a photograph of your kit or the end result.

**Which brings me to ice cream...?** One of the things we explored is what happens when you add salt and ice. If you have a digital thermometer you can take the measurement and what you see is that the temperature decreases. It is counterintuitive as you are adding salt

to ice and water and it is getting colder. Here the temperature plunges, so we start with making measurement, doing cooling curves, measuring what happens to temperature as a function of time etc.

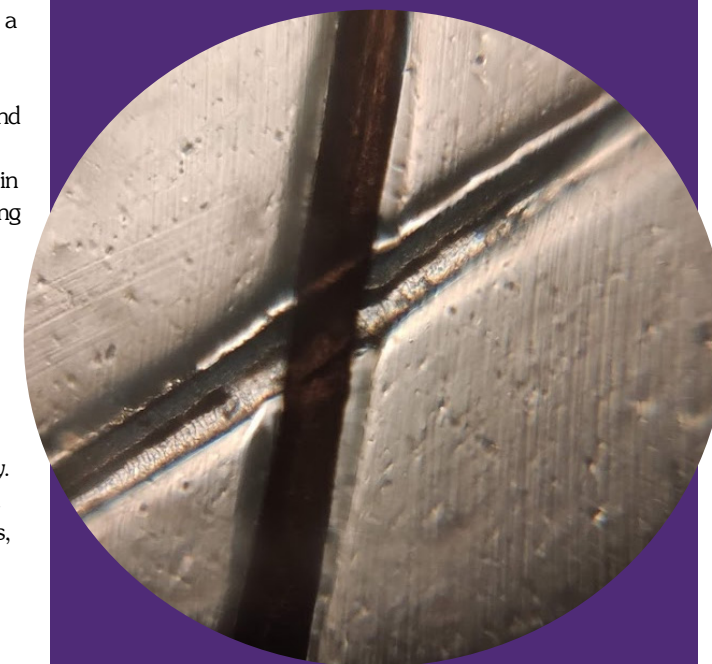
Again we used improvised apparatus – we used tic tac boxes as our sample holder for a number of our practicals. Once you have done that – why not do something silly, whimsical?

This is how you used to make ice cream.

You would churn cream sugar and eggs etc and you would cool it down with a mixture of salt and ice which you can get down to a minus 15 degrees. So now you share that with your family.

The idea that you share your practical with your wider family and community is incredibly important when thinking of teaching with public engagement. This is why I love the idea of students in labs tweeting their practicals to share out the joy and fun of doing it. What we got back was fabulous - we got absolutely amazing photos of students with their grandparents, parents, siblings all eating ice cream but also pets with interested cats and dogs all sampling.

I think sometimes there is not enough humour in some of our practicals - everything is very serious and there is not enough time to goof around and have some fun with it, to think laterally. We thought we should have a certain amount of edible silliness. We asked our students to make sugar glass – they grow crystals, and then they can make glass and then pulled sugar glass. It is neat and wacky and you can eat it.





### How was the testing phase – it must have been fun?

Absolutely – I went into a mad period of hyper focus where my family wanted to throttle me, I kept leaving solutions and bit and pieces lying around the house.

The other thing is having a mobile phone and this has become a crucial tool in the lab. We are uncomfortable with phones in the lab, but being able to do this at home and document it with your phone adds another dimension. One of the things you can do for example is film bubbles in a pan of water as it warms up. And you do see the most extraordinary things if you have a phone and take slo mo video and see this extraordinary bubble that rise up from the bottom, then expand and then collapse and disappear – it is something that once you start looking at things like that you begin to see the world in a different way. For a lot of our students with the right kind of guidance we can open up a different way of thinking about and viewing the world.

Initially I tested a bunch of things and presented to my colleagues and I started talking to other scientists and other chemistry department's teaching fellows across the country and a lot of positive feedback came back. We did a lot of testing over the summer and then we assembled the boxes.

### The box artwork is gorgeous

It was my colleague Mark Miodownik who asked how we are were going to decorate the boxes. We were in the pandemic, some of our students were isolated, they were incredibly frustrated and some could not come to the department. What we wanted to do was tell them 'this is our gift to you'. By putting the design on the box it was an attempt to personalise it. With the expansion of the dept. one of the consequences some of the really intimate friendships and atmosphere has sort of been diluted, we don't know each other as well. So this was kind of a way to address this emotional side, to say 'here is this beautiful gift'.

The artwork was done by the artist in residence at the Plastic Innovation hub, Ruby Wright who designed it while lying in a muddy field in Devon. I would send her picture of bits for the kit and she assembled this beautiful thing to fit around a box of photocopier paper.

### This really was a way of engaging students on the doorstep.

That was exactly the intention – we distributed these simply by handing them over to students scheduled to visit the department with good social distancing. There were many students self isolating, so I ride a bike with a trailer and so I did about 10 or 12 runs carrying boxes to halls of residents – I went as far as Stratford to ensure everyone had one.

### It wasn't all plain sailing though?

This year was bumpy, for some students it was really hard and lonely. I don't want this to be romanticised as we did have problems.

The big problem was sending the boxes abroad. For Europe for the most part they got there without trouble, except one to

Switzerland got there late March/early April. The boxes to China and Vietnam had big logistical problems.

We had the idea that every week there would be an activity and we would talk about it etc and as the boxes did not arrive, we had to let things slip, eventually the deadlines were gone and a lot of students let things slide. By the time we got to Xmas there was a backlog and there was a bit of panic and students were not as well supported with the week to week feedback and commentary we would have like to have given. This is something we hope for this year we can avoid as we don't have to ship the boxes and we can really support the students.

**Feedback from students is the Post Graduate Teaching Assistants (or Magic Elves) were heavily relied upon and very much appreciated.** The elves were absolutely essential – we had a whole team of lab elves, PGTA support elves – between the online forums and face to face online we were able to provide a lot of help.

There were a lot students who did not get in touch and who were distanced, and this is a real problem. The big challenge to how to we maintain and rebuild that sense of community and regular contact.

**How did you manage to get all this equipment together in the middle of a pandemic?** One of things is that I wanted things as simple and as cheap as possible – with an eye on the overall budget, but also with view to do as many things as possible. This is not a UCL idea. This is an idea for anyone and this should run in schools. We have this sense that we should have fancy equipment but live in a golden age where measuring equipment is available for peanuts. For me the go to place was Ebay. You can go and get a fancy pH meter commercial laboratory meter it will cost you £20-25 maybe £100 for a desktop one. But do we really care above exact values? We are not dealing with data that will have courtroom or commercial significance. What we want is a solid reliable measurement which will give a scientific basis that we need. If the pH is 7.2 and the reading gives us 6.9 then we can live with that. Actually this is really important

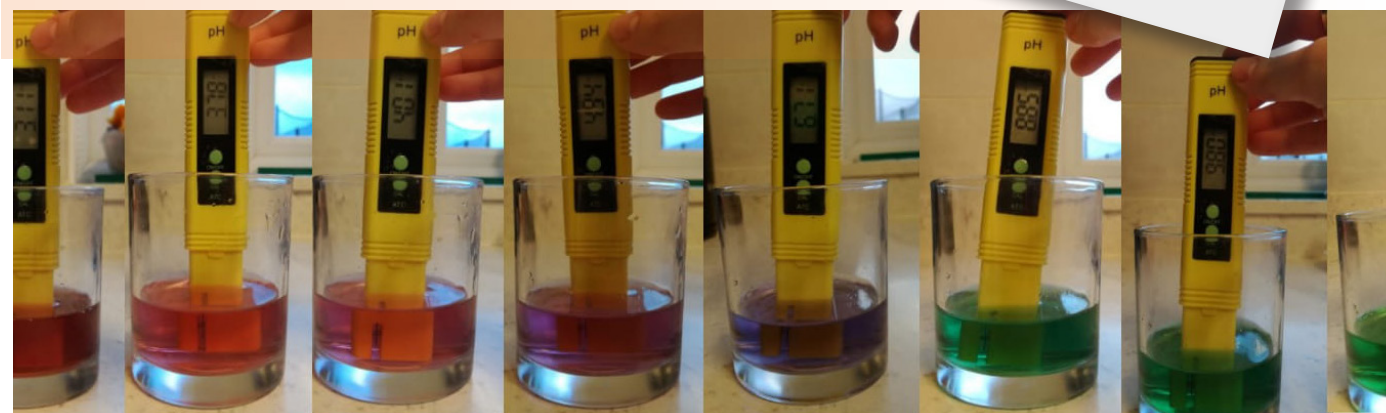
## Natalia Sanchez Castro

### MSci Biochemistry

There is no doubt not being able to regularly walk into a lab was one of the biggest disappointments of taking a practical course in a pandemic world. Having said this, it was eye-opening to see just how many of the core principles behind the theory we learned could be replicated at a smaller scale with mostly household items. The realisation that I had taken so many everyday objects for granted, without ever considering the science behind them, soon hit me.

My favourite experiment was using red cabbage to make a functional pH indicator, and I have since developed a much greater appreciation for this vegetable. I'll admit, things didn't always go smoothly. It's hard to put into words the frustration of buying household ingredients you don't use, waiting for crystals to grow in your fridge and evacuating your kitchen after the overwhelming stench of boiling vinegar fills the room – all in the same week. Despite the ups and downs, Lab14 was an opportunity I was very grateful to have. In any case, it was an excellent way to put the pomegranate salad dressing hiding in pantry to good use.

Natalia pictured sampling ice cream with two of her three brothers. Cabbage pH scale below.



Low pH <-----> High pH

– we have to get across how we live with doubt and uncertainty. Measurement is hard, understanding the world is hard and difficult. So what you have to do is do something that makes the measurement then you have to think and ask how reliable it is. How good it is – does it fit with the theory?

I wanted to build in a certain amount of sense of 'your not using something fancy – maybe you can't rely on it completely' so why not go and check. Are you not sure your scales work? Well how much does a 50p coin weigh? You know companies sell flour in 1kg – so you can check. The idea of improvisational and dealing with an uncertain world is something we could really capitalise on.

We don't want students to go through the motions – what gets me out of bed in the morning is that I might learn something, that there might be something 'neat' to be found. And this idea of an adventure playground in a box was the ethos.



Ice cream photo by Enrico Contreras, BSc  
Bioprocessing of New Medicines

### Meet: Ruby Wright

Lab 14 Box designer

Ruby Wright is an illustrator based in London.

She has been artist in residence for UCL's Plastic Waste Innovation Hub and sketcher in residence for Refugee Tales and is now working on her first picture book.

Visit:  
[www.rubywright.com](http://www.rubywright.com)  
Instagram  
(@rubywrightlino)



Read Daren Caruana, Christoph Salzmann and Andrea Sella's home based science manifesto published in Nature, August 2020

Caruana, D.J., Salzmann, C.G. & Sella, A. Practical science at home in a pandemic world. Nat. Chem. 12, 780–783 (2020). <https://doi.org/10.1038/s41557-020-0543-z>



# Heike Munro

BSc Biochemistry

## LastGen calling

It feels amazing to have survived this incredible and strange year, which was also my first year at UCL as a biomed undergraduate.

If it had not been for university lessons and an amazing and incredibly supportive student WhatsApp group, I am not sure how I would have survived all the other challenges thrown at me (breakdown of long-term relation, kids school issues, financial risks, prison-like existence due to lockdown etc).

Learning has always given me a tremendous joy - I know what you are thinking...but think about it, would I otherwise still do it at my age?

Even when some lessons were maybe less inspiring, being able to share this with my fellow students made that not only bearable but gave a strong sense of belonging. I cannot express the amount of gratitude to this amazing student body who has welcomed me so warmly despite the age difference.

Lab14 was another big part of getting me through this year. Wow, was that daunting to receive that box and basically told here is the manual - get on with it! However, the fear was short lived as I soon discovered the elves - magical creatures. Much love your way! With their support and a few, hmmm probably several, calls to the Bar chat room for support, I managed to undertake the experiments. Some even with sensible or at least recognisable result.

A hurdle of needing too many hands to handle all the equipment and taking photos resulted in a positive twist: my children got involved and Lab14 became our Sunday entertainment - my son being especially keen on the cakes and ice cream while my daughter and I had fun with Lego.

In addition, I learned even more the incredible power of kindness. So, thank you so much for all of you for making this challenging year a great year!



From top to bottom:

Lego was using LED photodiode, transparent/pink glass light refraction french fries, b/w salt grains through microscope, gold nuggets sugar glass, Santa Claus soap, Heike's son trying the ice cream and Heike

# Winnie Sae-Seung

BSc Chemistry with Management Studies

Winnie spoke with Chem News from her home in Bangkok, where she spent her first undergraduate year. Winnie outlined some of the highlights, challenges, and how she is helping improve Lab 14 for the future.

My first thought when the box arrived was that it was much bigger, I expected a much smaller lab kit. And you can see they really put a lot of thought into it. The box itself had the lab 14 artwork around it, which was a really nice touch rather than it arriving in a cardboard box, you can see that the people behind it they really did try to make it as nice as it could be.

When I opened it some things were familiar: kitchen scale, pipettes and other things we have seen before. But I also saw a lot of unfamiliar equipment, like a mechanical pipette, (which is a pretty cool piece of equipment to own), a thermocouple (which we used frequently) and a fold-able microscope which was very interesting. I also enjoyed diffraction grating film which is this little piece of plastic that did cool things with light - so all in all it was really fun to go through the contents.

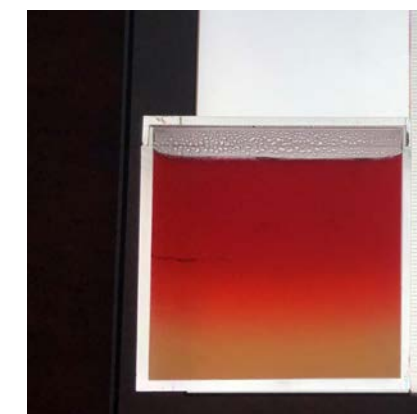
There were some experiments that were reminiscent of what I did at school - the heat capacity for instance is quite standard. But there is also some really interesting experiments I haven't seen before, that we could do safely at home. The saponification experiment really stood out to me, we mixed oil, caustic soda, and water - and you, somehow through the magic of organic chemistry, end up with a bar of soap. Though I was a bit hesitant to touch it because if I had done something wrong this could be a very corrosive bar of soap!

The kits helped with learning to schedule your time, as alongside online learning and navigating the theory, you had to find a way to fit in the practicals. Some things took 10-15 minutes, but others were quite time intensive. For example, the home titration took me a couple of hours for one trial, and that became tough to manage as there was 4 titrations overall. So learning to manage time and slot them in could be a little difficult. And of course some experiments don't turn out the way you want them to, some did not quite work, but taking into account the circumstance that is a home lab packed in a box, you can't really fault lab 14 for that!

I will be working with Dr Liz Munday and Dr J.L. Kiappes ((Associate Lecturers (Teaching)) over summer to help develop the Shikimic acid practical. The acid is extracted from star anise, and then that extract is used in a titration and a paper chromatogram to allow us to figure out if there is actually any Shikimic acid in our star anise extract. It took me about 3 plus hours to do the titration the first time and the chromatogram did not show up like it was supposed to, so I am hoping to help refine this for people who faced similar issues.

The titrations, for me, were one of the parts of lab 14 that I was most engaged with, as it reminded me of being in an actual lab, as it is a more traditional kind of experiment.

My top tips for lab 14 success is not to leave everything to the last minute. It is tempting, as you need to schedule everything, but if you leave it all for the April deadline it will become a lot of work and a lot of unnecessary stress. Try your best to engage with the experiments - it is natural you won't like everything that is in the manual, but give it a shot, it might surprise you.



From top to bottom:  
An epsom salt crystal shown through polarizing film  
the gel diffusion experiment  
Lego colorimeter,

## Meet: Liz Munday

Lab 14 Coordinator

Dr Liz Munday is an Associate Lecturer (Teaching) in Organic Chemistry and the Synthetic Laboratories. She started at UCL in July 2020, prior to which she worked as a Teaching fellow in Organic Chemistry at the University of Reading. She carried out her PhD at the University of St Andrews under the supervision of Prof. Andrew Smith, before which she carried out her MChem degree at the University of Oxford.





# Letizia Filippi

BSc Biochemistry

Dr Sella set up an inspiring product launch campaign for the Lab 14 kits, and there was a great buzz of excitement surrounding their release. I picked up my Lab 14 kit with a couple of biochemists staying at my accommodation, and we unpacked the boxes together. I remember that, even at the time, we noted how well put-together the kit was, but it wasn't until we had completed the last practical that we truly realised just how well. With around 10 pieces of "lab" equipment we were able to do over 25 experiments each exploring a different chemical principle.

After the initial excitement, the experiments weren't always smooth sailing. While the experiments varied in difficulty, often the science was straightforward and explained clearly within the lab manuals (although occasionally a practical would require further research). I felt a little intimidated to post questions on the forum so, when an experiment wouldn't quite work, I often repeated it multiple times, changing certain elements based on further research I did. This was very time consuming, and on occasion a short experiment would take me a couple of days. While, in hindsight, this was a great learning method and conceptually I did learn a lot, the first half of the academic year felt overwhelming, and I often felt behind. It was quite late into the year that I realised that it wouldn't be held against us to post a question on the forum.

The Professors and the "Lab 14 elves" are all genuinely lovely and eager to help (I truly don't know how, but all my questions were answered in under 24 hours). The forum is a safety net that really changed my perspective of Lab 14: it allowed me to enjoy the practical that had been set, focus on the chemistry and not worry too much about the actual results.



Above: Growing Crystals – Making Rochelle Salt  
Below: Failed attempts



While the forum is a great resource, I also often asked course mates for advice, which was a lot of fun since this often resulted in social occasions (or as much of a social occasion as was permitted under the COVID restrictions - and which were often hosted on zoom).

During A-Levels, the experiments were often poorly explained, done quickly and used apparatus and chemicals that I lacked regular access to. The childhood chemistry sets made up of cheap "test tubes" and "chemicals" were distant memories and science, for me, had started to feel inaccessible. What I loved most about Lab 14 was that it reminded me of science's universality - that with a tic-tac packet, water, salt, a thermocouple... and a Lab-14 manual, a chemical principle could be observed in my kitchen.

Lab 14 was an overwhelmingly positive experience, I would recommend you to get as involved as possible, and have fun!



## Faculty Education Awards

The Lab 14 Team received the MAPS Faculty Team Awards for Excellence.

The UCL Team are:

Andrea Sella  
Christoph Salzmänn  
Daren Caruana  
Liz Munday  
Helena Wong  
Hannah Shalloo  
Sabrina Simoncelli  
Miranda Molloy  
Harry Li  
Rebecca Chagoury  
Sergio Garcia Busto  
Alice Henley  
Catherine Webley  
Manish Trivedi,  
Manni Yang,  
Benji Thoma  
Omri Tau  
Belen Sola Barrado  
Panagiotis Fikas  
Minyan Lyu  
Jasper Fairchild  
Saeed Said  
Alan Philcox  
Ruby Wright

and from outside of UCL  
Aidan Kerrigan, Jack Dalglishby  
and Martin Whitworth.

## Sebastian Szkudelski

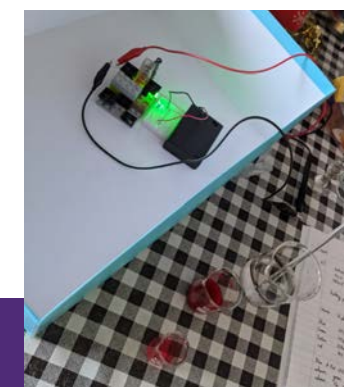
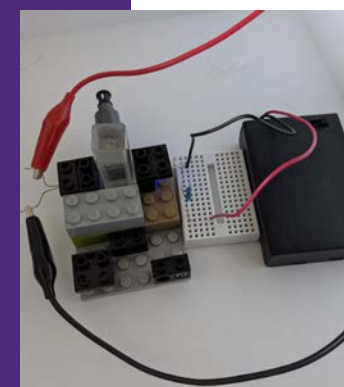
MSci Natural Sciences

With the academic year at its end, this is the perfect time to reflect on one of my most memorable experiences, lab 14, a box of goodies filled with everything needed to perform over 20 different experiments. Lab 14 allowed me to improve my lab skills, ranging from setting up my own makeshift Lego spectrophotometer to mastering the micropipette, there was something for everyone.

My favourite experiment involved extracting and purifying shikimic acid due to how involved the practical was and how it also relied on previous practical's along with the skills learnt from them. The satisfaction of everything working out in the end felt amazing.

One piece of advice I would give to the incoming first years is to not give up and have fun, there will be some experiments which won't work on your first go like my struggles with making edible glass but with practice it will work, and the results will be worth it. Most importantly remember to have fun, remember that you can repeat the experiments several times and experiment with different volumes and temperatures, maybe substitute some reagents and see what happens.

To conclude I had lots of fun with lab 14 and I look forward to working in the real lab next year.



Left: Lego spectrometer

Bottom: Packing 'elves' Claire Gacki & Martyn Towner





# Michael Chan

MSci Chemistry

I think the most enjoyable part of the lab kit, weirdly enough, has been making and learning from mistakes. For example, in one experiment, I had to titrate curcumin with sodium hydroxide. To extract the curcumin solution, I heated and filtered a solution of turmeric and water. During the extraction process, I accidentally boiled off all the water and burnt the turmeric, leaving my kitchen smelling heavily of turmeric for an entire week. In another, baking a cake seemed straightforward enough but, even after following the instructions, my cake came out a flat dry mess. In fact, it looked more like a biscuit than a cake. After checking with the thermocouple, I realised the actual temperature of the oven was much higher than the temperature shown on the oven display.

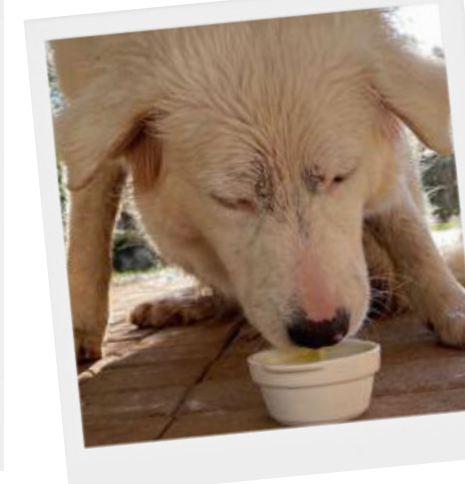
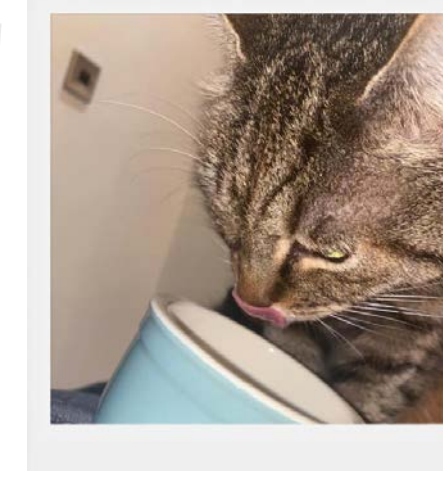
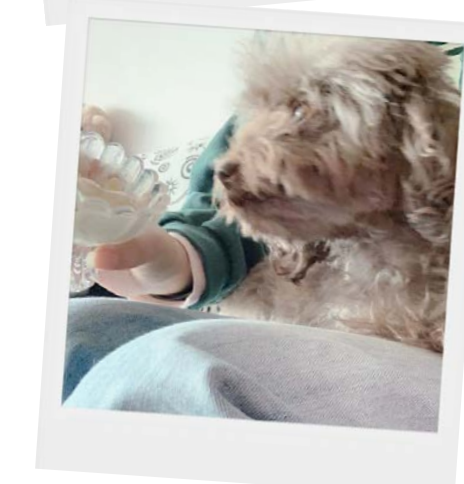
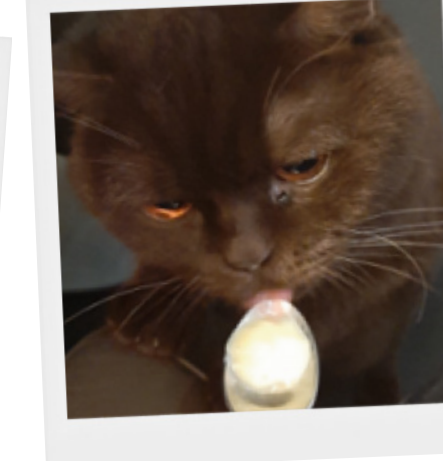
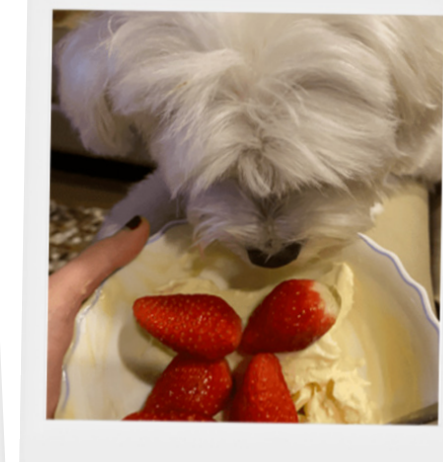
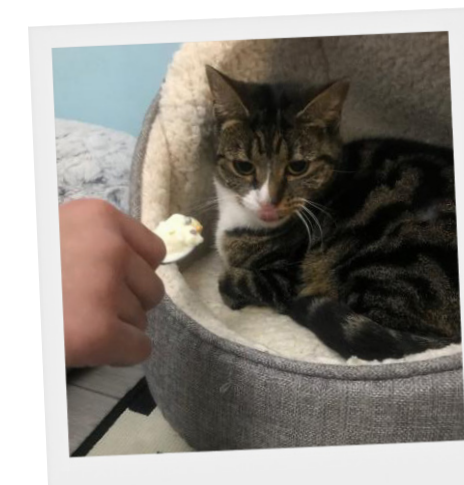
One of my favourite experiments involved measuring diffusion coefficients of food colouring. After setting up containers of gelatine – the top half with food colouring and the bottom half without, it was possible to measure the diffusion coefficient of each food colouring by taking photos at regular intervals. The coefficient itself is a measure of the rate of diffusion. Although a simple experiment, I was excited to see how far the food colouring had moved each time I opened the fridge.

I was slightly sceptical of the home lab kits at first. However, I have thoroughly enjoyed carrying out all the experiments and showing my results to my family. I have also learnt a lot: about my oven and about measuring accurately, from self-calibrating a pH meter to making DIY volumetric flasks. For incoming first years, note that there are a lot of interesting experiments that need to be done so, I advise you to manage your time well in order to complete Lab 14.



Top to Bottom Left to right: Michael, weighing brine, Crème brûlée, diffusion experiment, refraction of laser, milky water, synthesising sodium acetate, 2nd attempt at baking a cake.  
Below: left to right: red cabbage pH 3.22, pH6.37, pH 4.42, pH 10.01

**“We thought we should have a certain amount of edible silliness.”**





# Research Highlights

## Designer Aluminium Precursors for the Inkjet Printing of Electrical Circuits

Dr Caroline E. Knapp, EPSRC New Investigator Award



Dr Knapp was awarded an EPSRC New Investigator Award grant, which support individuals who hold an academic lectureship position, have not previously led an academic research group or been the recipient of a significant grant.

Printed electronics are becoming integrated into every part of modern-day life, from light-emitting diodes, to solar cells and printed biosensors such as wearable electronics. The flexible electronics market alone is predicted to be valued at \$74 billion by 2030. Whilst the technology already exists to manufacture large-scale flexible electronics, by way of the environmentally

friendly, roll-to-roll industrial processes which employ inkjet printing, currently the metal inks that are employed have their limitations. The patterning of molten metals is incompatible with affordable flexible materials, including renewable eco-friendly plastics or paper, this mismatch is due to, in part, the high melting point of metals (often over a thousand degrees) and the deformation temperature of a range of plastic, paper or fabric materials being considerably lower (ca. 100 – 200°C). Current techniques used in the production of printed electronics are time consuming and expensive multi step-techniques that require the use of toxic chemicals. These state-of-the-art techniques require metal flakes/particles to be ‘melted’ together, resulting in contaminants between layers, which reduce overall conductivity of the metal.

An obvious solution to this problem is the use of specially designed inks, containing small molecules that can be printed into any desired pattern onto any material, and then be thermally ‘activated’ at low temperatures, in order to convert them to conductive metal. This project aims to design and synthesise new small molecules to improve the performance of existing printing technologies. These would provide a tuneable alternative to the current industrial nanoparticle inks based on silver or copper whose activation temperatures are too high for printing onto many materials. In addition, understanding how the structure of a small molecule can influence its ability to act as a precursor to the metal is challenging, and gaining insight will enable us to adjust thermal activation temperatures, such that after printing, it can yield highly conductive metal.

Aluminium metal is earth abundant, boasts conductivity comparable to silver and copper and yet has never been used industrially to inkjet print conductive tracks. This is because suitable precursors do not exist, despite the rich field of synthetic aluminium chemistry. To overcome this problem, we propose to adapt our small molecule design to be better compatible with modern lower temperature deposition techniques. To reap the benefits of using printing techniques for device fabrication inks that will transform at low temperatures (affording compatibility with low-cost flexible materials) will be produced. This project will create a library of novel highly performing inks from aluminium which can be printed and sintered in air on low-cost flexible materials for incorporation into electronic devices.

Dr Fabrizia Foglia  
EPSRC Fellow

My research focuses to build an interdisciplinary research programme directed towards understanding how membrane morphology and local dynamics controls transport, and therefore how best tailoring and designing nanostructures to optimise performance and in general membrane nanotechnology. This relates to fields as diverse as energy and fuel cells, gas and/or chemical separation, and desalination applications, while it can be also extended to nanotechnology and biomedical applications. I primarily use and develop advanced neutron techniques to progress a fundamental understanding and, therefore, resolve molecular-level assembly mechanisms and pathways from a structural and dynamical point of view.



Dr José Marin-Beloqui  
UMA Fellow

**This newsletter we bid a sad farewell but send huge congratulations to PDRA researcher, Dr José Marin-Beloqui, who is off to start his new University of Málaga Fellowship in Spain. We find out about what he’s been up to at UCL as a PDRA and his future plans.**

**Tell us a little bit about your academic journey on the way to UCL.**

I did my first degree in the south of Spain in Málaga. After that, I moved to Tarragona, in northeastern Spain where I was at a chemistry research centre doing material science focus. Here, most of my colleagues were synthetic organic chemists, a big change to what I do now! Then, I moved to London for a 1 year PDRA position with Dr Saif Haque at Imperial college. This was only a short contract, and I wanted to stay in London, so I came to UCL to work with Dr Tracey Clarke. I’ve now been here 4 years and 4 months. It has gone so fast! I was checking some of the

Sandeep Kumar Padamati  
Marie Curie Fellow

Sandeep Kumar Padamati recently won the prestigious Marie-Curie Individual Fellowship to work with Prof. Katherine Holt, in the Department of Chemistry, UCL. He started his fellowship at the start of January 2021 in the middle of lockdown, so it was quite a few weeks before he even stepped foot in the department! Originally from India, Sandeep completed his Masters in Chemistry from University of Hyderabad in 2012. After which he pursued a PhD at the University of Groningen, Netherlands under the guidance of Prof. Wesley R Browne, and defended in 2017.

His PhD research work was primarily focussed on transition metal catalysts in oxidation studies, using iron, manganese and nickel catalysts with terminal oxidants such as H<sub>2</sub>O<sub>2</sub>, NaOCl, and O<sub>2</sub>. During which he has gained expertise in tracking the transient intermediates using spectroscopic tools; in particular Raman spectroscopy helped him hugely to identify the reaction intermediates.

After completion of his PhD, he moved to Université Grenoble Alpes, in France to work with Dr. Carole Duboc and Dr. Vincent Artero on the project of hydrogen evolution using Ni-Fe complexes that act as biomimics

of the hydrogenase enzyme active site. After his first Postdoc, he moved to Prof. Romana Schihragl’s group at UMCG,

## Research Fellows in Focus

first files from my time at UCL and I couldn’t believe how old they were. It has been brilliant though, I have learnt a lot about building labs, doing research and Tracey has been really supportive with my next career steps.

**What kind of research have you been doing at UCL and what are you going to be working on in Spain?**

My research is all about trying to figure out why things happen. A lot of my experiments come about because someone has a material and we measure it and figure out how it works. It’s always more interesting if it’s a system that is hard to understand. I now have a fellowship of my own in Spain for 2 years. I’m going to be working on a lot of Raman spectroscopy as well as picosecond transient absorption spectroscopy, which will be new to the host lab. I’m going to be looking into the fundamentals of the molecules involved in organic electronic devices such as solar cells.

**What are some of your best memories from UCL?**

The Christmas quiz! I only went to two of them but they were so much fun and we even won one, though most of the credit has to go to Jordan, one of our former PhD students. How he knew all of those random facts no one else knew! I’ve had the chance to do a lot of good research at UCL and really focus on doing experiments and looking at some exciting systems. I’ve met a lot of good people, both friends and career-wise and had

Netherlands in 2019 to work on functionalized nanodiamonds for observing the reactive oxygen species (ROS) generated in cells, using diamond magnetometry techniques.

Currently, Dr. Padamati is combining his experience in electrocatalysis and in functionalising diamond by working on the surface modification of Boron Doped Diamond (BDD) with metal oxides, such as MnO and CeO<sub>2</sub> by using electrodeposition methods and also Atomic Layer Deposition in collaboration with Prof. Chris Blackman. He is using these materials to perform electrochemical CO<sub>2</sub> reduction using electrocatalytic methods, determining the product distribution using <sup>1</sup>H NMR and catalyst stability using Raman Spectroscopy.

Another of his projects is to study the solvated electrons that are formed by the UV light irradiation on BDD, and he is constructing the spectrometer in collaboration with Dr. Michael Parkes. In summary, the project aim is to understand how the properties of diamond and transition metal catalysts can be combined for enhanced conversion of CO<sub>2</sub> into valuable chemicals such as CO and formic acid.



the chance to get involved in several committees, such as for the Chemistry, Light and Dynamics theme and for the PDRAs.

**What are you looking forward to at your new institute?**

As my new institute is in the south of Spain, it’s going to be super hot, I’m going to melt! But it’s a really nice region because you can be swimming in the sea and see the mountains. It’s also not far from Sierra-Nevada, the snow mountain, that you can go skiing in. I’m terrified about going right now! It has been a rollercoaster with the fellowship application and it’ll be tough starting again, but I’m also very excited about all the new possibilities with the lab and the independence I’ll have with the fellowship.

**If you had some had some advice to past on to postdocs to make the most of their time at UCL, what would it be?**

Start writing. Fellowships, grants, papers... It all takes a long time and the more you write the better you get. Ask other people, particularly who don’t know your research area, to read what you’ve written. If you can pass your knowledge to someone who doesn’t know the topic it’s a good sign for the grant. Get involved with the PDRA Committee and their activities – this is an excellent opportunity for networking and to meet people.



# Ultrafast Laser Spectroscopy

with Photons from the Infrared to the Extreme Ultraviolet

Prof. Helen Fielding

Light is essential for life.

For example, light is key to photosynthesis and vision. Light is also important in technology, such as in nanoscale optoelectronic devices. Developing a molecular-level understanding of light-induced processes is crucial for the rational design of new light-activated materials to address important challenges currently facing society, such as harnessing solar energy efficiently and developing new tools for disease diagnosis and therapeutics. Professor Helen Fielding, together with colleagues Professors Ivan Parkin and Geoff Thornton, Drs Tracey Clarke, Rebecca Ingle, Giorgio Volpe and Mike Parkes, has been awarded a £1.2M Strategic Equipment grant from the EPSRC to establish a unique, state-of-the-art, laser facility (Fig. 1) providing femtosecond light pulses over a wide range of energies, from the infrared (IR) to the extreme ultraviolet (EUV), to improve our fundamental understanding of light-induced processes.

They will achieve this by using a bottom-up approach to study systems across the complexity scale, from isolated gas-phase molecules to proteins, nanoparticles, soft materials and solids, for applications ranging from bioimaging and therapeutics to solar energy materials. Experiments will employ a single spectroscopic technique – femtosecond time-resolved photoelectron spectroscopy (TRPES) – in molecular and ion beams, liquid-microjets and on surfaces, complemented by femtosecond transient absorption spectroscopy (TAS), femtosecond stimulated Raman spectroscopy and multi-photon microscopy.

Gas-phase TRPES measurements of neutral molecules are carried out in the Fielding

Right: Fig. 1. The new ultrafast laser system at the heart of the new Ultrafast Laser Facility is a Coherent Astrella one-box Ti:Sapphire amplifier that generates 9 mJ pulses of 800 nm light at 1 kHz with 30 fs pulse duration. The output is split to pump 3 optical parametric amplifiers (providing wavelengths from 20 nm – 190 nm), a harmonic generator (400/266/200 nm) and a KM Labs XUUS high harmonic generation system to generate EUV pulses (62-35 nm).

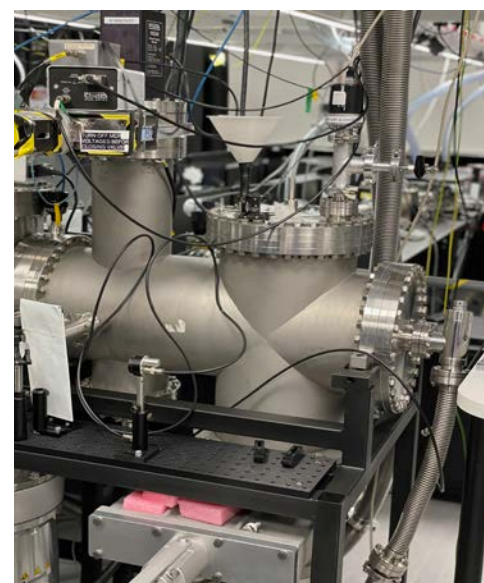
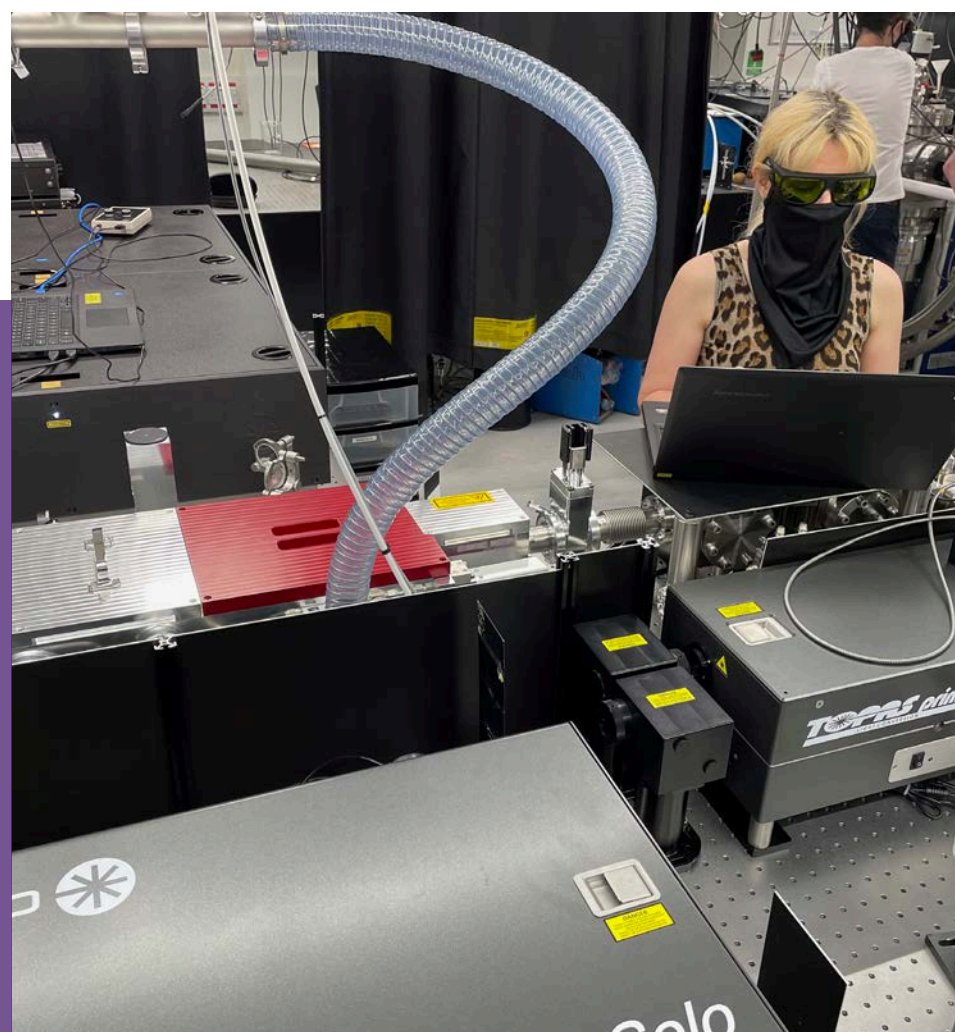


Fig. 2(a) Molecular-beam velocity map imaging photoelectron spectrometer,



Fig 2(b) electrospray-ionisation velocity map imaging photoelectron spectrometer,

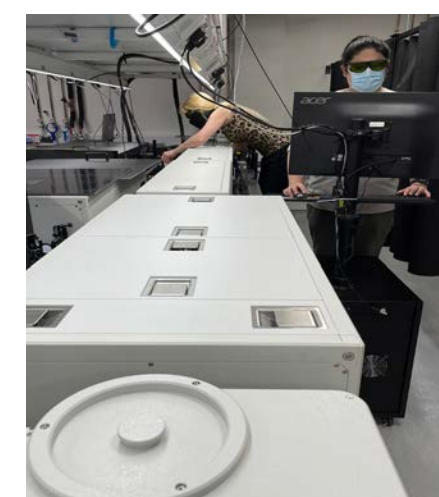
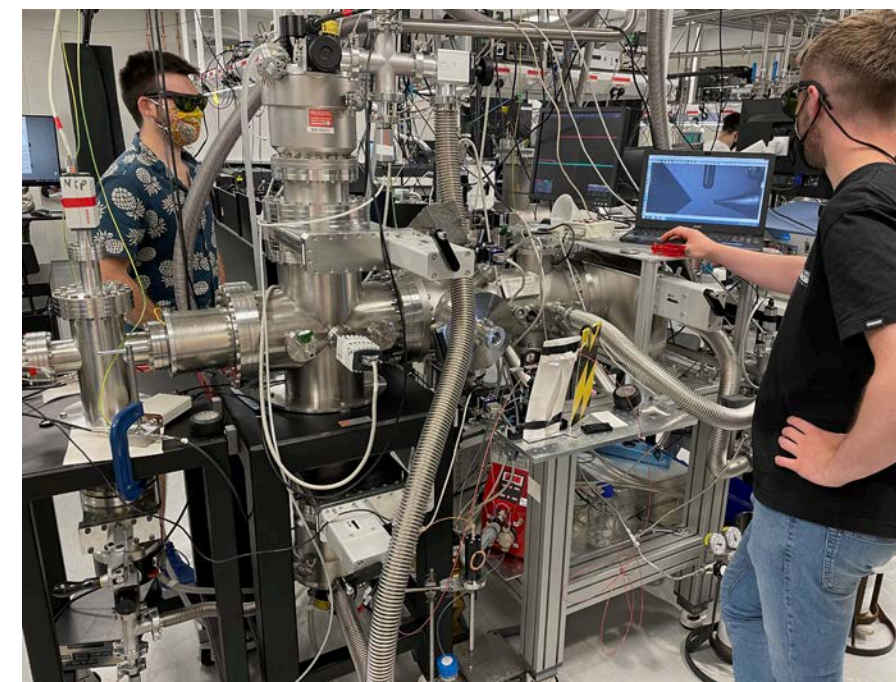


Fig 2(c) liquid-microjet magnetic-bottle time-of-flight photoelectron spectrometer,

Fig2(d) UHV hemispherical photoelectron analyser for surface science,

Fig 2(e) TAS/FSRS facility

Group's molecular beam velocity-map imaging photoelectron spectrometer that is equipped with an Amsterdam pulsed valve to transfer liquid or solid samples into the gas-phase (Fig. 2a).<sup>1</sup> Gas-phase TRPES measurements of ions are carried out in the group's electrospray-ionisation velocity-map imaging spectrometer that can transfer large molecules, e.g. protein chromophores, into the gas-phase in their deprotonated forms (Fig. 2b).<sup>2</sup> Solution-phase PES/TRPES measurements are carried out in the group's liquid-microjet magnetic bottle photoelectron spectrometer that has the capability for recirculating small volumes of liquids (Fig. 2c).<sup>3</sup> Surface TRPES measurements are carried out in collaboration with the Thornton group in an ultrahigh vacuum apparatus equipped with a hemispherical photoelectron analyser (Fig. 2d).<sup>4</sup>

The Fielding, Clarke, Ingle and Parkin groups will undertake complementary TAS and FSRS measurements (Fig. 2e), the Volpe group will exploit the laser system to develop the capability for multiphoton microscopy experiments using their existing microscope facilities and the Ingle group will establish the capability for two-dimensional electronic spectroscopy. The experimental toolkit available is unparalleled!

The new ultrafast laser facility is currently being exploited to develop a bottom-up approach for the rational design of new bioluminescence emitters. A detailed understanding of how molecular structure and biological environment control the brightness and colour modulation of bioluminescence emitters will enable us to design new probes for advanced imaging applications. Professors Helen Fielding, Jim Anderson and Graham Worth were awarded £1.4M funding from EPSRC to use synthetic organic chemistry, femtosecond TRPES and computational chemistry to probe the electronic structure and relaxation dynamics of the emitters that lie at the heart of bioluminescent systems, in the gas-phase, in micro-solvated environments, in aqueous solution and in enzymes. This work builds on earlier work from these groups,<sup>5</sup> and they plan exploit their new knowledge to design new bioluminescent emitters for multicolour, n-IR bioluminescence imaging.

The facility will also be exploited for TRPES measurements on a wide range of molecular systems as part of a recently awarded EPSRC Programme Grant investigating Ultrafast Photochemical Dynamics in Complex Environments. This project is a collaboration between Professors Helen Fielding and Graham Worth (UCL), Professor Andrew Orr-Ewing FRS (PI) and Dr Tom





Fig. 3 A triple celebration for the Fielding Group: Joey Broughton (front right with red cap) won the 2021 Ewing Prize for the best Physical Chemistry 3rd year PhD student talk, Will Fortune (lying down) won the 2021 Physical Chemistry poster prize at the 2nd year PhD poster competition and Pria Dobney (6th from the left) was awarded a 1st class MSci degree!

Oliver (University of Bristol), Professors Mark Brouard and Claire Vallance (University of Oxford), Professor Jon Marangos (Imperial College) and Dr Basile Curchod (Durham University).

Although moving all their equipment, from their old labs (121/122) to LG32 in the new Photon Science Science Hub during the second half of 2020 was made rather long and challenging by the pandemic, the future is looking very exciting for the Fielding Group.

The Ultrafast Laser Facility is open for collaborations with members of the UCL Chemistry Department, the wider UCL community and researchers from other UK Universities or from Industry. Anyone wishing to find out more should email Helen Fielding ([h.h.fielding@ucl.ac.uk](mailto:h.h.fielding@ucl.ac.uk)) and the Facility Manager, Dr Julia Davies ([julia.davies@ucl.ac.uk](mailto:julia.davies@ucl.ac.uk)).

#### References

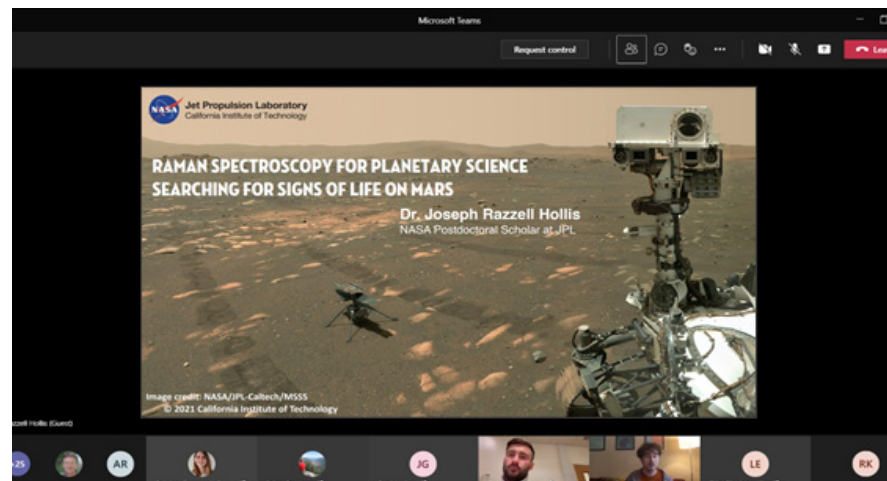
1. Fielding, H. H. & Worth, G. A. Using time-resolved photoelectron spectroscopy to unravel the electronic relaxation dynamics of photoexcited molecules. *Chem. Soc. Rev.* **47**, 309–321 (2018).
2. Henley, A. & Fielding, H. H. Anion photoelectron spectroscopy of protein chromophores. *Int. Rev. Phys. Chem.* **38**, 1–34 (2019).
3. Henley, A., Riley, J. W., Wang, B. & Fielding, H. H. An experimental and computational study of the effect of aqueous solution on the multiphoton ionisation photoelectron spectrum of phenol. *Faraday Discuss.* **221**, 202–218 (2020).
4. Tanner, A. J. *et al.* Polaron-adsorbate coupling at the TiO<sub>2</sub> (110)-carboxylate interface. *J. Phys. Chem. Lett.* **12**, 3571–3576 (2021).
5. Patel, A. M. *et al.* Shining light on the electronic structure and relaxation dynamics of the isolated oxytocin anion. *Phys. Chem. Chem. Phys.* **22**, 19022–19032 (2020).

## Chemistry Light & Dynamics Group

The Chemistry, Light and Dynamics Group (CLD) holds weekly seminars which provide space for our members to present, highlight work happening within the department, and regularly host distinguished invited speakers. The sessions are organised by a small team of postdocs and PhD students aiming to promote links between research groups at UCL while exposing students and staff to frontier research both from within UCL and from other institutions. The research groups currently constituting the CLD are those of Tracey Clarke, Helen Fielding, Tim Hele, Rebecca Ingle, Steve Price, David Rowley, Sabrina Simoncelli, Geoff Thornton, Graham Worth and Martijn Zwijnenberg. Indeed, the CLD has continued to grow year-on-year and further additions are always welcome!

The move to online talks has been taken in the CLD's stride, with the group's activities continuing in earnest on our new home of MS Teams. Special sessions this academic year included Women's Day, LGBTQ+ in STEM, Chemistry and Light Theme departmental seminars and several further invited talks (making full use of the potential to hear regularly from overseas speakers!). One of many highlights was the seminar by Dr. Joseph Razzell Hollis (Jet Propulsion Laboratory, California, USA) about some of the recent research by the Perseverance rover on Mars.

Weekly coffee mornings also help to maintain connection, even virtually, and these will continue throughout the summer before the seminar series returns in September. To join the CLD please sign up to the mailing list at <https://www.mailinglists.ucl.ac.uk/mailman/listinfo/cld-seminars> and keep up to date via the Teams page at <https://bit.ly/3CZKXgI>. We hope to continue to improve and expand the series over the coming year; if you are a PhD student or postdoc in the Chemistry and Light theme and want to contribute, please join the committee. It looks great on your CV! To do so, please email [cld-committee@ucl.ac.uk](mailto:cld-committee@ucl.ac.uk).



## Designer Nanopores for Portable Sensing of Diagnostic Proteins

Yongzheng Xing, Adam Dorey, Stefan Howorka



Stefan Howorka

The ongoing Covid-19 pandemic has dominated world events for the past two years. Amidst the chaos, the pandemic has united scientific researchers globally to collaborate on a single goal, to understand and ultimately overcome this deadly virus. The speed at which the SARS-CoV-2 virus spread around the world has highlighted the necessity of fast, sensitive and portable diagnostic devices. A key milestone in the history of the pandemic was the rapid sequencing of the SARS-CoV-2 genome, achieved using nanopore technology commercialized by Oxford Nanopore Technologies. Current nanopore sequencing is tailored to accommodate thin lengths of single-stranded DNA. In order to expand the range of sensing to larger molecules such as proteins and antibodies, there is a need for newly custom designed large-diameter nanopores.

Nanopore sensing relies on the passage of an ionic flow or current, through the pore lumen. As analytes pass through the pore this current signal is briefly blocked, giving a characteristic blocking profile that is dependent on the analytes size and shape. Existing protein-based pores have lumen sizes in the range of 1 to 5 nm, making them excellent sensors for small organic molecules, polymers, nucleic acids, and small proteins. However, the shortage of wider lumen pores has been a long-standing barrier in the application of portable and electrical sensing of larger proteins and protein complexes of significant biomedical and scientific interest.

To overcome this challenge, Dr. Yongzheng Xing from UCL Chemistry has created a series of functional nanopores with unprecedented lumen widths ranging from 5 to 30 nm.

The pores have been designed and constructed using DNA technology as conventional protein nanopores cannot be easily engineered to such sizes. By exploiting Watson-Crick

base pairing, DNA strands were predictably folded using a modular origami strategy into pores of well-defined sizes and polygonal geometries (see image). Dr. Adam Dorey from UCL Chemistry carried out a comprehensive electrical characterization of these nanopores, highlighting their compatibility with sensor platforms including the MinION kits from Oxford Nanopore Technologies, which have so far solely been used for DNA sequencing.

Rapid antibody detection will play a continued role in the coming months and years as a determination of SARS-CoV-2 immunity. As such, the DNA nanopores were modified with antibody-specific molecular receptors placed within the nanopore lumen. DNA nanotechnology simplifies this process in comparison to laborious site-specific modifications required for modification of biological protein pores. The modified DNA nanopores could detect two kinds of antibodies, an anti-biotin antibody, and a diagnostically important anti-SARS-CoV-2 spike protein antibody. Determinations of binding kinetics at the single molecule level were calculated and showed excellent agreement with ensemble measurements.

In summary, this research has generated a new rational design strategy to build large functional nanopores with precisely-defined shapes and sizes unachievable with current protein-based pores. This method will advance nanopore sensing techniques and widen the breadth of applications in biophysical and biomedical research and potentially provide a new toolkit to fight the current and any future pandemics.

The detailed methods and techniques from this work have been filed as a patent(s) and the research results are in review with Nature Nanotechnology.



## RSC Summer Bursary Student Lauren Cook describes her summer in Tim Hele's group

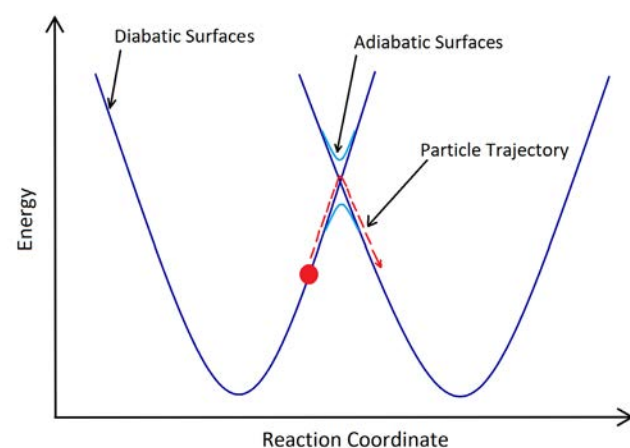
In the world of lockdowns and online learning, it seemed the opportunities for summer research were few and far between. I was delighted to obtain funding through the RSC undergraduate research bursary program to complete an eight-week summer research project with Dr Hele. In his first-year teaching at UCL, Dr Hele had made quite an impression on me through the quantum mechanics content taught in the third year 'Concepts in Computational Chemistry' module. Quantum mechanics has been a passion of mine, much to the surprise of my fellow coursemates, and is why I chose computational and coding optionals in the third year.

My project involves coding an algorithm to describe how photoexcited molecules change with time, known as the MInt algorithm. This algorithm should describe how both the electronic and nuclei move when a molecule has interacted with light and vitally, how molecules can 'jump' between electronic surfaces. This is known as non-adiabatic dynamics and is crucial to processes that occur in solar cells and LEDs. Computational models that can help increase the efficiency of renewable energy sources, by predicting what materials are of interest for optical applications, are sought after.

As the mid-June start date approached, I became quite nervous (but excited) at the prospect of coding this algorithm. My previous coding experience was very limited to a GCSE in computing and an introductory scientific programming module. Upon starting the project, I was put at ease by Dr Hele and found his enthusiasm for the work very infectious. As the MInt algorithm is very complicated, I started with a more straightforward version of the algorithm for dealing with simpler model systems. Once I had gained some confidence, I started coding the MInt algorithm. There were many challenging aspects of the code, particularly treating the behaviour of the electrons in the system and ensuring that energy was conserved properly in the run. I had to do a lot of

troubleshooting as I went to check everything was working as intended, as well as compare the results to those from another algorithm.

I have loved working on my project so far, although being remote from my bedroom is not quite how I pictured my first research project. Supervision via Zoom with Dr Hele has been enjoyable and aids in understanding the complex maths. Hints delivered by email have helped me to develop my problem-solving skills and social meetings with the group have made me feel part of the team, despite not yet having met in person! I look forward to the next 4 weeks of my project, focused more on testing the algorithm in the different systems it was developed for.



## Remote summer internships in the Chudasama Group

I am grateful to have had the opportunity to work with two excellent and very talented UCL undergraduates over summer 2020 in remote projects (Kristina Kostadinova and Clóna McMahon). It was naturally disappointing to us all that the summer internships could not take place in-person, but we wanted to make the most of the opportunity. To do this, we decided on trying to achieve the ambitious goal of publishing reviews in the areas of tyrosine modification and cysteine protecting groups. I was really pleased with how Kristina and Clóna responded, and stepped up to this significant challenge with great support from Peter Szijj and Dr Richard Spears. It was a pleasure to explore the science in these areas, have in-depth conversations and to even use it as an opportunity to think about new research avenues. The review Kristina worked on has been published in *Organic & Biomolecular Chemistry* (*Org. Biomol. Chem.*, **2020**, 18, 9018-9028), and the review Clóna worked on is currently under review in *Chemical Society Reviews*. I am very proud of Kristina and Clóna, as well as Peter and Richard, for all their efforts on these reviews; I really enjoyed working with them all.

Kristina commented:

*"I worked as a remote summer student in Prof. Chudasama's group after my second year and it has been amongst my most cherished experiences at UCL."*

*We worked on a review on the topic of tyrosine bioconjugation and I was responsible for writing up the initial draft, which included reading and organising a wide breadth of literature, as well as selecting the articles to be included in the review. This was extremely valuable as it allowed me to hugely improve my writing skills and my approach to working with scientific articles. I started appreciating the literature more critically and to pay more attention to the experimental methods, comparing and evaluating them. The analysis provided me with second-hand research experience, which will be helpful in my career development in academia. In addition, I gained insight into the process of publication. In the end, this summer internship also gave me the incredible opportunity – especially for a second-year student to publish a review article I co-authored."*

*The most interesting thing about this internship was being part of a group doing cutting-edge research in the field of protein bioconjugation. I was personally supervised by Prof. Chudasama and one of his PhD students, Peter Szijj, who were extremely supportive and patient, correcting all of my drafts, mentoring me through all the difficulties and teaching me all of these invaluable skills, while at the same time giving me enough room to work independently. For the first time, I also had the opportunity to see the dynamics of a research group, present*

*my progress on the group meetings and discuss ideas with my colleagues, thereby practicing teamwork and interpersonal skills. Most importantly, I had a wonderful time and I really enjoyed the work as the internship allowed me to build new connections. Everyone was very friendly, welcoming, and I still keep in touch with some of the people I worked with."*

*I am very thankful to Prof. Chudasama for giving me the incredible opportunity to work in his group and, together with Peter, for teaching me so much and supporting my development. I have grown more and more passionate about protein bioconjugation and now I am looking forward to continuing my studies with a master's or PhD project in the field."*

Clóna commented:

*"Last summer I undertook a remote summer project in the Chudasama Group. As an in-person lab project could not be done, a project which could be carried out entirely remotely was devised. For this project, I wrote and researched a literature review about cysteine protecting groups for use in solid-phase peptide synthesis and other related reactions."*

*Over the course of the project, I gained experience reading and analysing scientific literature, which was invaluable when it came to writing up a literature review for my MSci project this year. This project afforded me the opportunity to independently explore an area of chemistry in depth that really interested me. I came to understand how the field had developed over time, its key issues, and the research that is currently being done. It was especially interesting to work with researchers carrying out research in the field. I enjoyed my time on the project so much that I carried out my MSci project in the same field, investigating a novel cysteine protecting group for use in solid-phase peptide synthesis. The work that I did over the summer laid a great foundation for this project. It was also very rewarding to work as part of a research group, and I had the opportunity to present to and get advice from the other members of the Chudasama group."*

*I am especially grateful to Professor Vijay Chudasama for the opportunity to carry out a project in his group and for his supervision and guidance, and to Dr Richard Spears for helping to devise the project and his supervision, help and encouragement throughout the course of the project. I thoroughly enjoyed my time doing this project and I learnt a lot of skills which I have been able to apply to subsequent work. I am looking forward to beginning my PhD in Chemical Biology this autumn!"*

Despite the constraints of remote working and social distancing, the department was able to host undergraduates for summer internships & bursaries.

# Summer Training



Summer Students left to right: Kristina Kostadinova and Clóna McMahon and RSC Bursary recipient Lauren Cook



# Alumni Matters

## Obituaries

### Prof. Ronald J. Gillespie

August 21 1924 – February 20 2021

Ron Gillespie, one of our distinguished alumni from the Ingold era, has died in Canada at the age of 96.

He came as a student to the Chemistry Department in 1942 when it was evacuated to Aberystwyth. In 1944, when the Department returned to London he joined Professor Ingold's team who were using a multidisciplinary approach to tackle the problem of aromatic nitration with nitric/sulfuric acid mixtures. People like Bunton and Minkoff were using kinetic measurements, Millen was using spectroscopy, Goddard was isolating stable intermediates, and Ron was investigating the cryoscopy of nitric acid in sulphuric acid. The group converged on the solution that the reaction took place by the attack of the nitronium ion intermediate, NO<sub>2</sub><sup>+</sup>, on the aromatic ring.

Sulfuric acid has a melting point of 10°C. With nitric acid in solution it shows a depression of the m.p. corresponding to a van't Hoff factor of 4 as the HNO<sub>3</sub> is protonated and dissociates.



Jim Millen showed that the Raman spectrum of the the nitronium ion, O=N<sup>+</sup>=O was similar to that of the isoelectronic carbon dioxide molecule O=C=O, and Dan Goddard isolated nitronium salts such as the perchlorate, NO<sub>2</sub><sup>+</sup> ClO<sub>4</sub><sup>-</sup>, and tetrafluoroborate NO<sub>2</sub><sup>+</sup> BF<sub>4</sub><sup>-</sup>. People who were present still remember Ingold's superb lecture summarising this work, when, half way through, he nonchalantly brought out from his waistcoat pocket a sample of nitronium perchlorate, which chemists expected to be very explosive.

In 1949, Ingold published this work in a series of 22 papers which occupied 285 pages in the Journal of the Chemical Society. Ingold wrote all the papers but not all carried his name. Ron Gillespie was named as the author of five of the papers which carried his name alone or with a research student. Ingold gave him the manuscripts to check before they were submitted, with the invitation to make any changes he wished, but Ron made none.

In 1949, Ron was awarded a Ph.D. and was appointed as an Assistant Lecturer without having made a formal application, and before he was awarded the Ph.D. Life was less formal in those days. With his own research students he studied the properties of other solutes in sulfuric acid, using further techniques such as electrochemistry. In 1953 he was awarded a Commonwealth Fund Fellowship to enable him to work in the USA at Brown University with Robert Cole to determine the dielectric constant of sulfuric acid.

On a personal note, I was at that time an Assistant Lecturer at Battersea Polytechnic. Ted Hughes phoned me and asked me to drop in for a chat. The upshot was that I moved back to UCL to take over Ron's lectures, with Don Llewellyn, to Intermediate and 1st MB students.

Back at UCL and teaching bonding theory, Ron became dissatisfied with the model involving hybrid orbitals, and he teamed up with Ron Nyholm to develop the alternative approach of Valence Shell Electron Pair Repulsion (VSEPR) which assumes that the bonding and non-bonding electron pairs surrounding the central atom will space themselves out to minimise their mutual repulsion. Together, they wrote a now-classic article in Quarterly Reviews,<sup>1</sup> Ron Gillespie dealing with compounds of the main group metals and Ron Nyholm covering the transition metals, and the subject soon found a place in undergraduate courses and textbooks.

These topics of sulphuric acid solutions and of the VSEPR model, and their expansions into super acid solutions and the LCP (Ligand Close Packed) model were to define Ron Gillespie's later career.

The UK was still suffering from wartime restrictions and the support for research and for modern equipment was difficult to obtain. Ron Gillespie and Ron Nyholm were trying to raise the money to buy an NMR spectrometer, and on a visit to Varian in California, Ron Gillespie stopped at McMaster University in Hamilton, Ontario, to see Arthur Bourns who had spent some time at UCL. McMaster was then a small Baptist college but had aspirations to expand into a major research university. They offered Ron his own NMR and Raman spectrometer, research support from the NRC, and double his UK salary, and despite Ingold's persuasion, he moved to McMaster in 1958 and remained there for the rest of his career. Ron Nyholm is widely regarded as leading the post-war renaissance of inorganic chemistry in Britain, and Ron Gillespie did much the same for Canada.

E.A. (Peter) Robinson (see the photograph) had just completed his Ph.D. with Ron and moved with him to McMaster to help to set up Ron's research group and to continue postdoctoral work on sulphuric acid solutions. In 1961, Peter moved to Toronto and spent all his subsequent career in Canada but continued to work closely with Ron and much of their work was published jointly. Peter published a review of Ron's career and chemistry in 2000.<sup>2</sup>

In Canada, Ron continued working on sulfuric acid solutions, using cryoscopy, conductivity measurements, and Raman and NMR spectroscopy to identify the solutes which were formed. With this experience he extended the work to HF and HSO<sub>3</sub>F, which are stronger acids than H<sub>2</sub>SO<sub>4</sub> and need special techniques because of their corrosive nature. In particular, solutions of SbF<sub>5</sub> in HF or HSO<sub>3</sub>F had the highest known acidities and were termed superacids. Fluorosulfuric acid has the low melting point of -85°C which enables the site of protonation of solutes to be determined by NMR. George Olah exploited the use of HSO<sub>3</sub>F/SbF<sub>5</sub> ("magic acid") to generate carbocations and for this work was awarded the Nobel Prize in Chemistry in 1994.



Ron Gillespie (right) and Peter Robinson (left) at Saskatoon, Canada, ca. 1959.

Gillespie used the superacid media to generate a large number of new polyatomic compounds of main group elements such as I<sub>4</sub><sup>2+</sup>, Br<sub>3</sub><sup>+</sup>, S<sub>4</sub><sup>2+</sup>, Se<sub>4</sub><sup>2+</sup>, Se<sub>10</sub><sup>2+</sup>, Te<sub>6</sub><sup>2+</sup>, S<sub>3</sub>N<sup>+</sup>, Sn<sub>6</sub>N<sub>4</sub><sup>2+</sup>. By X-ray crystallography he determined the structures of many of these compounds, and many were novel. Similarly new fluorocations of xenon and krypton fluorides were prepared and their structure studied by <sup>19</sup>F NMR.

Ron avoided administration and devoted his time to research and teaching. He published some 330 research papers, books on VSEPR, and undergraduate text books which modernised the teaching of chemistry.

He was a keen traveler. He met his wife Madge on a hiking trip to Switzerland in 1949; and they were married in 1950; they had two daughters, Ann and Lynn. They enjoyed camping and skiing trips, and Ron had a Wayfarer dinghy which he sailed on Lake Ontario. They were both avid travellers, keen to experience different cultures, and spent sabbatical leave in England, France, Switzerland, New Zealand, Australia, and

India. Madge died in 2008, and in 2010 he married his second wife, Michelle. His character can be summed up in the words I heard used to introduce him when he was awarded a prize in Canada: "It is said that nice guys never win; Ron is exception which proves the rule".

When he was in England, Ron would come to the Lab Dinner. He funded a series of visiting lectures in the Department and the Gillespie Prize, which is still extant, which is awarded to one of our graduates who is proceeding to an inorganic Ph.D.

He was elected as a Fellow of the Royal Society of Canada (FRSC) in 1965, a Fellow of the Royal Society (FRS) in 1977, and made a member of the Order of Canada (OC) in 2007.

1. R.J. Gillespie and R.S. Nyholm, Quart. Revs. Chem. Soc., 1957, 11, 339.
2. E.A. Robinson, Coord. Chem. Revs., 2000, 197, 3.

**Alwyn Davies**



## Dr Michael D. Johnson

Mike had graduated at Southampton, and after a postdoc period with E.S.Lewis at the Rice Institute in USA he came to UCL as an ICI Fellow in 1959 and was appointed lecturer in 1962.

His work at UCL was initially on the mechanism of organic reactions, and covered reactions of quinoline derivatives, and electrophilic addition to alkenes.

In the course of a few years his interests moved to the reaction mechanism of metal-carbon bonds in both transition and main group metals, and in 1978 he published a review in *Accounts of Chemical Research* on his and related work on the reaction of electrophiles with  $\sigma$ -bonded organotransition-metal compounds.

He had a long series of papers on the alkylcobalt compounds, particularly the cobaloximes, which was accompanied by a substantial authoritative review with David Dodd on the organic compounds of cobalt(II). Bimolecular homolytic substitution at saturated carbon was then, and still is, a very rare phenomenon, but he showed that it could be observed in alkyl cobalt(II) cobaloximes and related compounds. This work was summarised in a second *Accounts of Chemical Research* article in 1983. The reaction can be induced intramolecularly in the reaction of radicals with but-3-enylcobaloximes, when it leads to the formation of cyclopropanes of potential as synthetic pyrethroid precursors.

He was very active in student affairs, through which he will be well remembered by past students. He was a senior treasurer of the Students' Union from 1967 to 1971 and was appointed Vice-Warden (under Denys Holland) of Max Rayne House from 1970 to 1973. On Denys's departure, he became Warden of both Max Rayne House and Ifor Evans Hall in 1973-4 and again in 1980-84.

He was also Chairman of the Bloomsbury Theatre Management Committee from its opening in 1967 to 1974 and

remained a member of that committee until 1984. He was treasurer of the college branch of the AUT (Association of University Teachers, and he claimed to have the distinction of



being a member of the Faculty Committee at Senate House for more than twenty years without ever having attended a meeting.

He had a strong social conscience and outside College he was University-appointed governor of Haverstock School, Chalk Farm, and founder and chairman of the Haverstock Housing Association which provided (and continues to provide) affordable rental accommodation for schoolteachers in the Borough of Camden.

He took early retirement in 1984 to follow his other interests in the writing and production of plays, short sketches, and comedy routines. In some of his plays, Departmental characters are clearly visible. He maintained strong contact with the college and up to a year ago he regularly attended lunches with his contemporaries. He had rapidly progressing dementia and succumbed to it in September 2021.

**Alwyn Davies**

## Prof. Michael Abraham

We are sad to report that Prof. Michael Abraham, Honorary Professor UCL Chemistry passed away on 19 January.

Mike was an eminent scientist and prolific author in the field of physical organic chemistry who has published about seven hundred papers.

His research focused on physical organic chemistry, especially as applied to environmental chemistry and medicinal/pharmaceutical chemistry. Mike developed the Abraham General Solvation Model. He was at the University of Surrey until 1988 and on leaving moved to UCL where he continued to be active in research up until the very end.

Mike was also a professional artist, and was involved in setting up many exhibitions. Mike was also very keen on classical music concerts especially chamber music.



## Thank you...

### Prof. E.A (Peter) Robinson



The department would like to thank Professor E. A. (Peter) Robinson (pictured right) who has kindly donated regularly over the years to the department and recently gave a very generous donation. Peter obtained his BSc in Chemistry in 1955 at UCL and stayed to complete a PhD in 1958 with Professor Ronald J. Gillespie, who at the time was an assistant lecturer. Peter recalls that having just completed his BSc being sent a note from the then Head of Chemistry, Sir Christopher Ingold FRS, asking to meet with him. During the meeting Sir Christopher Ingold told Peter that he would like him to continue after his BSc to do postgraduate work towards a doctorate and assigned him to work with Ronald Gillespie. The result of this was a very long partnership and friendship (66 years!) with Peter going with Gillespie to McMaster University as a postdoctoral fellow in 1958.

Peter's doctoral thesis (self-typed!) was entitled "Cryoscopic and Conductimetric Studies in Sulphuric Acid as a Non Aqueous Solvent" and extended to 569 pages with his PhD being awarded in 1958. Peter joined the University of Toronto faculty in 1961 as an Assistant Professor of chemistry before moving to create Erindale College (now University of Toronto, Mississauga), an entirely new "Off-Campus College" where Peter served as Professor, Associate Dean, Dean and finally Principal. Peter retired in 1998 and when fully retired returned to England where he currently lives and over the years enjoyed many visits from Ronald Gillespie. Professor Ronald Gillespie sadly passed away in February 2021.

#### Donations

A big thank you to all the kind people who have supported the department directly to help us to build on our international reputation for teaching, research, and to make a range of exciting activities possible. Your kind contributions have a direct impact upon our students and staff, and we are very grateful for it. We continue to provide an excellent education and training environment for undergraduate and postgraduate students in Chemistry and all staff are developing innovative methods to inspire and instruct. It is great to know that we have your support and assistance as we work to do this.



# Publications

Abdurahman A, **Hele TJH**, Gu Q, Zhang J, Peng Q, Zhang M, Friend RH, Li F, Evans EW, Understanding the luminescent nature of organic radicals for efficient doublet emitters and pure-red light-emitting diodes, *Nature Materials*, 2020, **19**, 1224-1229, 10.1038/s41563-020-0705-9.

Abfalterer A, Shamsi J, Kubicki DJ, Savory CN, Xiao J, Divitini G, Li W, MacPherson S, Gałkowski K, MacManus-Driscoll JL, **Scanlon DO**, Stranks SD, Colloidal synthesis and optical properties of perovskite-inspired cesium zirconium halide nanocrystals, *ACS Materials Letters*, 2020, **2**, 1644-1652, 10.1021/acsmaterialslett.0c00393.

Acosta-Gutierrez S, Bodrenko IV, Ceccarelli M, The influence of permeability through bacterial porins in whole-cell compound accumulation, *Antibiotics (Basel)*, 2021, **10**, 635, 10.3390/antibiotics10060635

Agarwal N, Thomas L, Nasrallah A, Sainna MA, Freakley SJ, Edwards JK, **Catlow CRA**, Hutchings GJ, Taylor SH, Willock DJ, The direct synthesis of hydrogen peroxide over Au and Pd nanoparticles: A DFT study, *Catalysis Today*, 2020, 10.1016/j.cattod.2020.09.001

Agote-Arán M, Kroner AB, Wragg DS, Sławiński WA, Briceno M, Islam HU, Sazanovich IV, Rivas ME, Smith AWJ, Collier P, Lezcano-González I, **Beale AM**, Understanding the deactivation phenomena of small-pore Mo/H-SSZ-13 during methane dehydroaromatisation, *Molecules*, 2020, **25**, 5048, 10.3390/molecules25215048

Aina AA, Misquitta AJ, **Price SL**, A non-empirical intermolecular force-field for trinitrobenzene and its application in crystal structure prediction, *The Journal of Chemical Physics*, 2021, **154**, 094123, 10.1063/5.0043746

Alotaibi AM, Promdet P, Hwang GB, Li J, Nair SP, Sathasivam S, Kafizas A, **Carmalt CJ**, **Parkin IP**, Zn and N codoped TiO<sub>2</sub> thin films: photocatalytic and bactericidal activity, *ACS Applied Material Interfaces*, 2021, **13**, 10480-10489, 10.1021/acsmami.1c00304

Alqahtani M, Kafizas A, Sathasivam S, Ebaid M, Cui F, Alyamani A, Jeong HH, Chun Lee T, Fischer P, **Parkin I**, Grätzel M, Wu J, A Hierarchical 3D TiO<sub>2</sub>/Ni nanostructure as an efficient hole-extraction and protection layer for GaAs photoanodes, *ChemSusChem*, 2020, **13**, 6028-6036, 10.1002/cssc.202002004

Amon A, Sener ME, Rosu-Finsen A, Hannon AC, **Slater B**, **Salzmann CG**, Preparation and structure of the ion-conducting mixed molecular glass Ga<sub>2</sub>I<sub>3,17</sub>, *Inorganic Chemistry*, 2021, **60**, 6319-6326, 10.1021/acs.inorgchem.1c00049

Anand M, Baletto F, Bugaev A, **Catlow R**, Claeys M, Conway M, Davidson M, Davies P, de Leeuw N, Eremin D, Fischer N, Hargreaves J, Hutchings G, Iyer J, Jain D, Jameel F, Kamali AR, Kondrat S, Kowalec I, Kraus P, Reece C, Réocreux R, Santos-Carballal D, Seavill PW, Shoji M, Sinev M, Sinha V, Stamatakis M, Uner D, Vojvodic A, Whiston K, Willock D, Wolf M, Yang B, Zhu B, Theory: general discussion, *Faraday Discussions*, 2021, **229**, 131-160, 10.1039/d1fd90030g

Anand M, **Beale AM**, Boronat M, Bowker M, Bugaev AL, Bukhtiyarov VI, **Catlow CRA**, Chansai S, Claeys M, Conway M, Davies PR, Edwards J, El-Kadi J, Eremin D, Fischer N, Guan S, Hargreaves JSJ, Hess C, Hutchings GJ, Jameel F, Reza Kamali A, Kondrat S, Lawes N, Lennon D, Li D, Morgan P, Oyarzun Aravena AM, Reece C, Reocreux R, Seavill PW, Sekine Y, Shoji M, Silverwood I, Sinev M, Smith C, Stamatakis M, Torrente Murciano L, Uner D, Weckhuysen BM, Whiston K, Wolf M, Yang B, Zeinalipour-Yazdi CD, Advanced approaches: general discussion, *Faraday Discussions*, 2021, **229**, 378-421, 10.1039/d1fd90032c

Ananikov V, Bugaev A, Chansai S, Claeys M, Conway M, Eremin D, Greaves M, Hess C, Hintermair U, Hutchings G, Jameel F, Kamali AR, Koehler K, Malkov A, Morgan P, Oyarzun Aravena AM, Seavill PW, Sinev M, Torrente Murciano L, Uner D, Whiston K, Williams CK, Wolf M, Dynamics: general discussion, *Faraday Discussions*, 2021, **229**, 489-501, 10.1039/d1fd90031e

**Anderson JC**, Bouvier-Israel E, Rundell CD, Zhang X, Asymmetric synthesis of piperidines using the nitro-Mannich reaction, *Tetrahedron*, 2021, **78**, 131821, 10.1016/j.tet.2020.131821

Arhangelskis M, **Bučar D-K**, Bordignon S, Chierotti MR, Stratford SA, Voinovich D, Jones W, Hasa D, Mechanochemical reactivity inhibited, prohibited and reversed by liquid additives: examples from crystal-form screens, *Chemical Science*, 2021, **12**, 3264-3269, 10.1039/d0sc05071g

Arulkumaran N, Lanphere C, Gaupp C, Burns JR, Singer M, **Howorka S**, DNA Nanodevices with selective immune cell interaction and function, *ACS Nano*, 2021, **15**, 4394-4404, 10.1021/acsnano.0c07915

Ashton TE, Baker PJ, Sotelo-Vazquez C, Footer CJM, Kojima KM, Matsukawa T, Kamiyama T, **Darr JA**, Stoichiometrically driven disorder and local diffusion in NMC cathodes, *Journal of Materials Chemistry A*, 2021, **9**, 10477-10486, 10.1039/d1ta01639c

Ayyala SK, Tsang JH, **Blackman C**, Covington JA, Comparative study of spin-coated and vapour deposited nickel oxides for detecting VOCs, *Proceedings of IEEE Sensors*, 2020, 10.1109/SENSOR547125.2020.9278881

Bacellar C, Kinschel D, Mancini GF, **Ingle RA**, Rouxel J, Cannelli O, Cirelli C, Knopp G, Szlachetko J, Lima FA, Menzi S, Pamfilidis G, Kubicek K, Khakhulin D, Gawelda W, Rodriguez-Fernandez A, Biednov M, Bressler C, Arrell CA, Johnson PJM, Milne CJ, Chergui M, Spin cascade and doming in ferric hemes: Femtosecond X-ray absorption and X-ray emission studies, *Proceedings of the National Academy of Sciences of the United States of America*, 2020, **117**, 21914-21920, 10.1073/pnas.2009490117

Bahou C, Szijj PA, Spears RJ, Wall A, Javaid F, Sattikar A, Love EA, **Baker JR**, **Chudasama V**, A Plug-and-play platform for the formation of trifunctional cysteine bioconjugates that also offers control over thiol cleavability, *Bioconjugate Chemistry*, 2021, **32**, 672-679, 10.1021/acs.bioconjchem.1c00057 **Bakewell C**, Magnesium hydrides bearing sterically demanding amidinate ligands: synthesis, reactivity and catalytic application, *Dalton Transactions*, 2020, **49**, 11354-11360, 10.1039/d0dt02523b

Barnes NG, Ahmed Mal Ullah AA, Ragazzon PA, Charafi N, Hadfield JA, Syntheses of Combretastatin A-4 and related stilbenes by using aqueous conditions, *ChemistrySelect*, 2021, **6**, 7082-7086, 10.1002/slct.202101960

Barnes NG, Nyandoro K, Jin H, **Macmillan D**, Rapid access to Asp/Glu sidechain hydrazides as thioester precursors for peptide cyclization and glycosylation, *Chemical Communications*, 2021, **57**, 1006-1009, 10.1039/D0CC07404G

Barnes NG, Parker AW, Ullah AAAM, Ragazzon PA, Hadfield JA, A 2-step synthesis of Combretastatin A-4 and derivatives as potent tubulin assembly inhibitors, *Bioorganic & Medicinal Chemistry*, 2020, **28**, 115684-115685, 10.1016/j.bmc.2020.115684

**Battaglia G**, The Effect of Glycans Steric Potentials on Virus Infectivity- the SARS-CoV-2 Case, *Biophysical Journal*, 2021, **120**, 329A, 10.1016/j.bpj.2020.11.2070

Beddoes CM, Gooris GS, **Foglia F**, Ahmadi D, Barlow DJ, Lawrence MJ, Deme B, Bouwstra JA, Arrangement of Ceramides in the Skin: Sphingosine Chains Localize at a Single Position in Stratum Corneum Lipid Matrix Models, *Langmuir*, 2020, **36**, 10270-10278, 10.1021/acs.langmuir.0c01992

Beine AK, Zeng F, **Negahdar L**, Palkovits S, Palkovits R, Optimization of the oxygen evolution reaction – Electrode development and kinetic investigations, *Chemie Ingenieur Technik*, 2020, **92**, 1289, 10.1002/cite.202055013

Bellany F, Tsuchiya Y, Tran TM, Chan AWE, Allan H, Gout I, **Tabor AB**, Design and synthesis of Coenzyme A analogues as Aurora kinase A inhibitors: An exploration of the roles of the pyrophosphate and pantetheine moieties, *Bioorganic & Medicinal Chemistry*, 2020, **28**, 115740, 10.1016/j.bmc.2020.115740

Bhide MA, Manzi JA, **Knapp CE**, **Carmalt CJ**, Synthetic and Structural Studies of Ethyl Zinc β-Amidoenates and β-Ketoiminates, *Molecules*, 2021, **26**, 3165, 10.3390/molecules26113165

Bhide MA, Mears KL, **Carmalt CJ**, **Knapp CE**, Synthesis, solution dynamics and chemical vapour deposition of heteroleptic zinc complexes via ethyl and amide zinc thioureides, *Chemical Science*, 2021, **12**, 8822-8831, 10.1039/d1sc01846a

Bieniek MK, Bhati AP, Wan S, **Coveney PV**, TIES 20: Relative Binding Free Energy with a Flexible Superimposition Algorithm and Partial Ring Morphing, *Journal of Chemical Theory and Computation*, 2021, **17**, 1250-1265, 10.1021/acs.jctc.0c01179

Bosse L, Mant BP, Schleier D, Gerlach M, Fischer I, Krueger A, Hemberger P, **Worth G**, Threshold Photoelectron Spectrum of Cyclobutadiene: Comparison with Time-Dependent Wavepacket Simulations, *The Journal of Physical Chemistry Letters*, 2021, **12**, 6901-6906, 10.1021/acs.jpcclett.1c01848

Brlec K, Davies D, **Scanlon D**, Surfaxe: systematic surface calculations, *The Journal of Open Source Software*, 2021, **6**, 3171, 10.21105/joss.03171

Brun J, Vasiljevic S, Gangadharan B, Hensen M, V. Chandran A, Hill ML, **Kiappes JL**, Dwek RA, Alonzi DS, Struwe WB, Zitzmann N, Assessing antigen structural integrity through glycosylation analysis of the SARS-CoV-2 viral spike, *ACS Central Science*, 2021, **7**, 586-593, 10.1021/acscentsci.1c00058

Bueno CZ, Apolinário AC, Duro-Castano A, Poma A, Pessoa A, Rangel-Yagui CO, **Battaglia G**, L-Asparaginase encapsulation into asymmetric permeable polymersomes, *ACS Macro Letters*, 2020, **9**, 1471-1477, 10.1021/acsmacrolett.0c00619

Burns JR, Introducing bacteria and synthetic biomolecules along engineered DNA fibers, *Small*, 2021, **17**, 2100136, 10.1002/sml.202100136

Büschges MI, Hoffmann RC, **Regoutz A**, Schlueter C, Schneider JJ, Atomic layer deposition of ternary indium/tin/aluminum oxide thin films, their characterization and transistor performance under illumination, *Chemistry – A European Journal*, 2021, **27**, 9791-9800, 10.1002/chem.202101126

Byrne C, Zahra KM, Dhaliwal S, Grinter DC, Roy K, Garzon WQ, Held G, **Thornton G**, Walton A, A combined laboratory and synchrotron in-situ photoemission study of the rutile TiO<sub>2</sub> (110) / Water Interface, *Journal of Physics D: Applied Physics*, 2021, **54**, 194001, 10.1088/1361-6463/abddfb

Caltagirone C, Draper ER, Hardie MJ, **Haynes CJE**, Hiscock JR, Jolliffe KA, Kieffer M, McConnell AJ, Leigh JS, An Area-Specific, International community-led approach to understanding and addressing equality, diversity, and inclusion issues within supramolecular chemistry, *Angewandte Chemie International Edition*, 2021, **60**, 11572-11579, 10.1002/anie.202015297

**Caruana DJ**, **Salzmann CG**, **Sella A**, Practical science at home in a pandemic world, *Nature Chemistry*, 2020, **12**, 780-783, 10.1038/s41557-020-0543-z

Carvalho da Fonseca AC, Matias D, Medeiros Geraldo LH, Leser FS, Pagnoncelli I, Garcia C, do Amaral RF, da Rosa BG, Grimaldi I, de Camargo Magalhaes ES, Coppola-Segovia V, de Azevedo EM, Zanata SM, Souza Lima FR, The multiple functions of the co-chaperone stress inducible protein 1, *Cytokine & Growth Factor Reviews*, 2021, **57**, 73-84, 10.1016/j.cytogfr.2020.06.003

Cassidy SS, Sanders DJ, Wade J, **Parkin IP**, **Carmalt CJ**, Smith AM, Allan E, Antimicrobial surfaces: A need for stewardship?, *PLoS Pathogens*, 2020, **16**, e1008880, 10.1371/journal.ppat.1008880

**Catlow CRA**, Concluding remarks: Reaction mechanisms in catalysis: perspectives and prospects, *Faraday Discussions*, 2021, **229**, 502-513, 10.1039/d1fd00027f

**Catlow CRA**, Wells P, Gianolio D, Synchrotron radiation techniques in catalytic science, *Physical Chemistry Chemical Physics*, 2020, **22**, 18745-18746, 10.1039/d0cp90186e

Chadwick A, **Catlow CRA**, A tribute to the scientific career of Neville Greaves: the Daresbury years, *Journal of Physics: Condensed Matter*, 2021, **33**, 320401, 10.1088/1361-648X/ac02e2

Chen S, Rowland S, Carr J, Storm M, Choy KL, **Clancy AJ**, The importance of particle dispersion in electrical treeing and breakdown in nano-filled epoxy resin, *International Journal of Electrical Power & Energy Systems*, 2021, **129**, 106838, 10.1016/j.ijepes.2021.106838

Choi Y, **Scanlon DO**, Lee J, Extending the performance limit of anodes: insights from diffusion kinetics of alloying anodes, *Advanced Energy Materials*, 2020, **11**, 2003078, 10.1002/aenm.202003078

Christopoulou G, Freibert A, **Worth GA**, Improved algorithm for the direct dynamics variational multi-configurational Gaussian method, *The Journal of Chemical Physics*, 2021, **154**, 124127, 10.1063/5.0043720

Churchill B, Acree Jr. WE, **Abraham MH**, Abraham model correlation for direct water-to-2,2,5,5-tetramethyloxolane solute transfer revisited, *Physics and Chemistry of Liquids*, 2020, **58**, 833-838, 10.1080/00319104.2019.1675161

**Clancy AJ**, Suter TM, Taylor A, Bhattacharya S, Miller TS, Brázdová V, **Aliev AE**, Chauvet AAP, **Corà F**, Howard CA, **McMillan PF**, Understanding spontaneous dissolution of crystalline layered carbon nitride for tuneable photoluminescent solutions and glasses, *Journal of Materials Chemistry A*, 2021, **9**, 2175-2183, 10.1039/d0ta11070a

**Clarke TM**, How to split an exciton, *Nature Energy*, 2020, **5**, 644-645, 10.1038/s41560-020-00689-2

Clayson IG, Hewitt D, Hutereau M, Pope T, **Slater B**, High throughput methods in the synthesis, characterization, and optimization of porous materials, *Advanced Materials*, 2020, **32**, 2002780, 10.1002/adma.202002780

Coates CS, Baise M, Schmutzler A, Simonov A, Makepeace JW, Seel AG, Smith RI, Playford HY, Keen DA, Siegel R, Senker J, **Slater B**, Goodwin AL, Spin-ice physics in cadmium cyanide, *Nature Communications*, 2021, **12**, 2272, 10.1038/s41467-021-22515-3

Colville BWF, **Powner MW**, Selective prebiotic synthesis of α-threofuranosyl cytidine by photochemical anomerization, *Angewandte Chemie International Edition*, 2021, **60**, 10526-10530, 10.1002/ange.202101376

Conboy D, Kielty P, Bear JC, **Cockcroft JK**, Farràs P, McArdle P, Singer RJ, Smith DA, Aldabbagh F, Ring-fused dimethoxybenzimidazole-benzimidazolequinone (DMBBQ): tunable halogenation and quinone formation using NaX/Oxone, *Organic & Biomolecular Chemistry*, 2021, **19**, 2716-2724, 10.1039/d1ob00032b



Coomber CE, **Porter MJ**, **Aliev AE**, Smith PD, **Sheppard TD**, Tuning reactivity in Pd-catalysed C(sp(3))-H arylations via directing group modifications and solvent selection, *Advanced Synthesis & Catalysis*, 2020, **362**, 5105-5115, 10.1002/adsc.202000726

Costa SIR, Choi Y-S, Fielding AJ, Naylor AJ, Griffin JM, Sofer Z, **Scanlon DO**, Tapia Ruiz N, Surface engineering strategy using urea to improve the rate performance of Na<sub>2</sub>Ti<sub>3</sub>O<sub>7</sub> in Na-ion batteries, *Chemistry – A European Journal*, 2021, **27**, 3875-3886, 10.1002/chem.202003129

**Coveney PV**, Computational biomedicine. Part 1: molecular medicine, *Interface Focus*, 2020, **10**, 20200047, 10.1098/rsfs.2020.0047

**Coveney PV**, Groen D, Hoekstra AG, Reliability and reproducibility in computational science: implementing validation, verification and uncertainty quantification *in silico*, *Philosophical Transactions of the Royal Society A: Mathematical, Physical, and Engineering Sciences*, 2021, **379**, 20200409, 10.1098/rsta.2020.0409

**Coveney PV**, Highfield RR, When we can trust computers (and when we can't), *Philosophical transactions. Series A, Mathematical, physical, and engineering sciences*, 2021, **379**, 20200067, 10.1098/rsta.2020.0067

**Coveney PV**, Hoekstra A, Rodriguez B, Viceconti M, Computational biomedicine. Part II: organs and systems, *Interface Focus*, 2021, **11**, 1-4, 10.1098/rsfs.2020.0082

Crovetto A, Xing Z, Fischer M, Nielsen R, Savory CN, Rindzevicius T, Stenger N, **Scanlon DO**, Chorkendorff I, Vesborg PCK, Experimental and first-principles spectroscopy of Cu<sub>2</sub>SrSnS<sub>4</sub> and Cu<sub>2</sub>BaSnS<sub>4</sub> photoabsorbers, *ACS Applied Materials & Interfaces*, 2020, **12**, 50446-50454, 10.1021/acsami.0c14578

Cui F, Zhang Y, Fonseka HA, Promdet P, Channa AI, Wang M, Xia X, Sathasivam S, Liu H, **Parkin IP**, Yang H, Li T, Choy K-L, Wu J, **Blackman C**, Sanchez AM, Liu H, Robust protection of III-V nanowires in water splitting by a thin compact TiO<sub>2</sub> layer, *ACS Applied Materials & Interfaces*, 2021, **13**, 30950- 30958, 10.1021/acsami.1c03903

Da Ros S, **Aliev AE**, del Gaudio I, King R, Pokorska A, Kearney M, Curran K, Characterising plasticised cellulose acetate-based historic artefacts by NMR spectroscopy: a new approach for quantifying the degree of substitution and diethyl phthalate contents, *Polymer Degradation and Stability*, 2020, 109420, 10.1016/j.polymdegradstab.2020.109420

Daley T, Opuni K, Raj E, Dent AJ, Cibin G, Hyde TI, **Sankar G**, Monitoring the process of formation of ZnO from ZnO<sub>2</sub> using in situ combined XRD/XAS technique, *Journal of Physics: Condensed Matter*, 2021, **33**, 264002, 10.1088/1361-648X/abfb91

Daskalakis S, Wang M, **Carmalt CJ**, Vernardou D, Electrochemical investigation of phenethylammonium bismuth iodide as anode in aqueous Zn<sup>2+</sup> electrolytes, *Nanomaterials*, 2021, **11**, 656, 10.3390/nano11030656

De Pace C, Marchello G, **Perez LR**, **Battaglia G**, Brownian Tomography of Biomolecules and Soft Polymer Assemblies, *Microscopy and Microanalysis*, 2020, **26**, 1024-1025, 10.1017/S1431927620016700

Decarolis D, Clark AH, Pellegrinelli T, Nachttegaal M, Lynch EW, **Catlow CRA**, Gibson EK, Goguet A, Wells PP, Spatial Profiling of a Pd/Al<sub>2</sub>O<sub>3</sub> Catalyst during selective ammonia oxidation, *ACS Catalysis*, 2021, **11**, 2141-2149, 10.1021/acscatal.0c05356

Dedman CJ, King AM, Christie-Olea JA, **Davies G-L**, Environmentally relevant concentrations of titanium dioxide nanoparticles pose negligible risk to marine microbes, *Environmental Science: Nano*, 2021, **8**, 1236-1255, 10.1039/d0en00883d

Dedman CJ, Rizk MMI, Christie-Olea JA, **Davies G-L**, Investigating the impact of cerium oxide nanoparticles upon the ecologically significant marine cyanobacterium, *Prochlorococcus*, *Frontiers in Marine Science*, 2021, **8**, 10.3389/fmars.2021.668097

Dey N, **Haynes CJE**, Supramolecular coordination complexes as optical biosensors, *ChemPlusChem*, 2021, **86**, 418-433, 10.1002/cplu.202100004

Di Maiolo F, **Worth GA**, Burghardt I, Multi-layer Gaussian-based multi-configuration time-dependent Hartree (ML-GMCTDH) simulations of ultrafast charge separation in a donor–acceptor complex, *The Journal of Chemical Physics*, 2021, **154**, 144106, 10.1063/5.0046933

Dietrich K, Jaensson N, Buttinoni I, **Volpe G**, Isa L, Microscale Marangoni Surfers, *Physical Review Letters*, 2020, **125**, 098001, 10.1103/physrevlett.125.098001

Dobrijevic D, Nematollahi LA, **Hailes HC**, Ward JM, pET expression vector customized for efficient seamless cloning, *Biotechniques*, 2020, **69**, 384-387, 10.2144/btn-2020-0101

Don CH, Shiel H, Hobson TDC, Savory CN, Swallow JEN, Smiles MJ, Jones LAH, Featherstone TJ, Thakur PK, Lee TL, Durose K, Major JD, Dhanak VR, **Scanlon DO**, Veal TD, Sb 5s<sup>2</sup> lone pairs and band alignment of Sb<sub>2</sub>Se<sub>3</sub>: a photoemission and density functional theory study, *Journal of Materials Chemistry C*, 2020, **8**, 12615-12622, 10.1039/d0tc03470c

Dong H, Butler KT, Matras D, Price SWT, Odarchenko Y, Khatry R, Thompson A, Middelkoop V, Jacques SDM, **Beale AM**, Vamvakeros A, A deep convolutional neural network for real-time full profile analysis of big powder diffraction data, *npj Computational Materials*, 2021, **7**, 74, 10.1038/s41524-021-00542-4

Douglas SP, Mrig S, **Knapp CE**, Frontispiece: MODs vs. NPs: Vying for the future of printed electronics, *Chemistry – A European Journal*, 2021, **27**, 10.1002/chem.202183161

Douglas SP, Mrig S, **Knapp CE**, MODs vs. NPs: Vying for the future of printed electronics, chemistry – *A European Journal*, 2021, **27**, 8062-8081, 10.1002/chem.202004860

Dover CM, Grinter DC, Yim CM, Muryn CA, Bluhm H, Salmeron M, **Thornton G**, Orientation of acetic acid hydrogen bonded to acetate terminated TiO<sub>2</sub>(110), *Surface Science*, 2020, **699**, 121628, 10.1016/j.susc.2020.121628

Duro-Castano A, Leite DM, Forth J, Deng Y, Matias D, Jesus CN, **Battaglia G**, Designing peptide nanoparticles for efficient brain delivery, *Advanced Drug Delivery Reviews*, 2020, **160**, 52-77, 10.1016/j.addr.2020.10.001

Dutta G, **Regoutz A**, Moschou D, Enzyme-assisted glucose quantification for a painless Lab-on-PCB patch implementation, *Biosensors and Bioelectronics*, 2020, **167**, 112484, 10.1016/j.bios.2020.112484

Qian E, Wadawadigi A, Zha O, Liu K, Dai J, Eddula S, Jiang C, Zhang A, Zhu S, Garcia E, Acreee Jr. WE, **Abraham MH**, Determination of Abraham model correlations for describing solute transfer into the methyl butyrate mono-solvent at 298 K, *Physics and Chemistry of Liquids*, 2020, **58**, 792-802, 10.1080/00319104.2019.1660983

Edeling W, Arabnejad H, Sinclair R, Suleimenova D, Gopalakrishnan K, Bosak B, Groen D, Mahmood I, Crommelin D, **Coveney PV**, The impact of uncertainty on predictions of the CovidSim epidemiological code, *Nature Computational Science*, 2021, **1**, 128-135, 10.1038/s43588-021-00028-9

Ellis-Gibblings L, Fortune W, Cooper B, Tennyson J, **Price SD**, Ionisation of PF<sub>3</sub>: absolute partial electron ionisation cross sections and the formation and reactivity of

dication states, *Physical Chemistry Chemical Physics*, 2021, **23**, 11424-11437, 10.1039/D1CP01328A

Engel J, Schwartz E, **Catlow CRA**, Roldan A, The influence of oxygen vacancy and Ce<sup>3+</sup> ion positions on the properties of small gold clusters, *Journal of Materials Chemistry A*, 2020, **8**, 15695-15705, 10.1039/d0ta01398f

Eom W, Lee E, Lee SH, Sung TH, **Clancy AJ**, Lee WJ, Han TH, Carbon nanotube-reduced graphene oxide fiber with high torsional strength from rheological hierarchy control, *Nature Communications*, 2021, **12**, 396, 10.1038/s41467-020-20518-0

Fallon KJ, Wijeyasinghe N, Leventis A, Marin-Beloqui JM, Toolan DTW, Al-Hashimi M, **Clarke TM**, Anthopoulos TD, Bronstein H, Tyrian purple: An ancient natural dye for cross-conjugated n-type charge transport, *Journal of Materials Chemistry C*, 2021, **9**, 4200-4205, 10.1039/d0tc05553k

Fang Z, Tian S, Li B, Liu Q, Liu B, Zhao X, **Sankar G**, VO<sub>2</sub>/ZnO bilayer films with enhanced thermochromic property and durability for smart windows, *Applied Surface Science*, 2020, **540**, 148414, 10.1016/j.apsusc.2020.148414

Farleigh M, Pham TT, Yu Z, Kim J, Sunassee K, Firth G, Forte N, **Chudasama V**, **Baker JR**, Long NJ, Rivas C, Ma MT, New bifunctional chelators incorporating dibromomaleimide groups for radiolabeling of antibodies with positron emission tomography imaging radioisotopes, *Bioconjugate Chemistry*, 2021, 10.1021/acs.bioconjchem.0c00710

**Foglia F**, **Clancy A**, Berry-Gair J, Lisowska K, Wilding M, Suter T, Miller T, Smith K, Demmel F, Appel M, Garcia Sakai V, **Sella A**, Howard C, Tyagi M, **Cora F**, **McMillan P**, Aquaporin-like water transport in nanoporous crystalline layered carbon nitride, *Science Advances*, 2020, **6**, eabb6011, 10.1126/sciadv.abb6011

**Foglia F**, Lyonnard S, Garcia Sakai V, Berrod Q, Zanotti J-M, Gebel G, **Clancy A**, **McMillan PF**, Progress in neutron techniques: towards improved polymer electrolyte membranes for energy devices, *Journal of Physics: Condensed Matter*, 2021, **33**, 264005, 10.1088/1361-648X/abfc10

Fowles DJ, Palmer DS, Guo R, **Price SL**, Mitchell JBO, Toward physics-based solubility computation for pharmaceuticals to rival informatics, *Journal of Chemical Theory and Computation*, 2021, **17**, 3700-3709, 10.1021/acs.jctc.1c00130

Francia NF, Price LS, Nyman J, **Price SL**, Salvalaglio M, Systematic finite-temperature reduction of crystal energy landscapes, *Crystal Growth & Design*, 2020, **20**, 6847-6862, 10.1021/acs.cgd.0c00918

Fu Z, Vogel A, **Zwijnenburg MA**, Cooper AI, Sprick RS, Photocatalytic syngas production using conjugated organic polymers, *Journal of Materials Chemistry A*, 2021, **9**, 4291-4296, 10.1039/d0ta09613j

Galdadas I, Carlino L, Ward RA, Hughes SJ, Haider S, **Gervasio FL**, Structural basis of the effect of activating mutations on the EGF receptor, *eLife*, 2021, **10**, e65824, 10.7554/eLife.65824

Galdadas I, Qu S, Oliveira ASF, Olehnovics E, Mack AR, Mojica MF, Agarwal PK, Tooke CL, **Gervasio FL**, Spencer J, Bonomo RA, Mulholland AJ, Haider S, Allosteric communication in class A β-lactamases occurs via cooperative coupling of loop dynamics, *elife*, 2021, **10**, e66567, 10.7554/eLife.66567

Galovic M, Erlandsson K, Fryer TD, Hong YT, Manavaki R, Sari H, Chetcuti S, Thomas BA, Fisher M, Sephton S, Canales R, Russell JJ, **Sander K**, **Arstad E**, Aigbirhio FI, Groves AM, Duncan JS, Thielemans K, Hutton B, Coles JP, Koepp MJ, NEST investigators, Validation of a combined image derived input function and venous sampling approach for the quantification of [<sup>18</sup>F]GE-179 PET binding in the brain, *NeuroImage*, 2021, **237**, 118194, 10.1016/j.neuroimage.2021.118194

Gentili A, **Volpe G**, Characterization of anomalous diffusion classical statistics powered by deep learning (CONDOR), *Journal of Physics A: Mathematical and Theoretical*, 2021, **54**, 314003, 10.1088/1751-8121/ac0c5d

Gheorghiu A, **Coveney PV**, Arabi AA, The influence of base pair tautomerism on single point mutations in aqueous DNA, *Interface Focus*, 2020, **10**, 20190120, 10.1098/rsfs.2019.0120

Gheorghiu A, **Coveney PV**, Arabi AA, The influence of external electric fields on proton transfer tautomerism in the guanine-cytosine base pair, *Physical Chemistry Chemical Physics*, 2021, **23**, 6252-6265, 10.1039/d0cp06218a

Gibson QD, Zhao T, Daniels LM, Walker HC, Daou R, Hébert S, Zanella M, Dyer MS, Claridge JB, **Slater B**, Gaultois MW, **Corà F**, Alaria J, Rosseinsky MJ, Low thermal conductivity in a modular inorganic material with bonding anisotropy and mismatch, *Science*, 2021, eabh1619, 10.1126/science.abh1619

Grande CA, Blom R, Middelkoop V, Matras D, Vamvakeros A, Jacques SDM, **Beale AM**, Di Michiel M, Anne Andreassen K, Bouzga AM, Multiscale investigation of adsorption properties of novel 3D printed UTSA-16 structures, *Chemical Engineering Journal*, 2020, **402**, 126166, 10.1016/j.cej.2020.126166

Greene MK, Chen T, Robinson E, Straubinger NL, Minx C, Chan DKW, Wang J, Burrows JF, Van Schaeybroeck S, **Baker JR**, **Caddick S**, Longley DB, Mager DE, Straubinger RM, **Chudasama V**, Scott CJ, Controlled coupling of an ultrapotent auristatin warhead to cetuximab yields a next-generation antibody-drug conjugate for EGFR-targeted therapy of KRAS mutant pancreatic cancer, *British Journal of Cancer*, 2020, **123**, 1502-1512, 10.1038/s41416-020-01046-6

Grinter DC, Allan M, Yang HJ, Salcedo A, Murgida GE, Shaw B-J, Pang CL, Idriss H, Ganduglia-Pirovano MV, **Thornton G**, Ce=O Terminated CeO<sub>2</sub>, *Angewandte Chemie International Edition*, 2021, **60**, 13835-13839, 10.1002/anie.202101771

Groen D, Arabnejad H, Jancauskas V, Edeling WN, Jansson F, Richardson RA, Lakhili J, Veen L, Bosak B, Kopta P, Wright DW, Monnier N, Karlshoefer P, Suleimenova D, Sinclair R, Vassaux M, Nikishova A, Bieniek M, Luk OO, Kulczewski M, Raffin E, Crommelin D, Hoenen O, Coster DP, Piontek T, **Coveney PV**, VECMAtk: a scalable verification, validation and uncertainty quantification toolkit for scientific simulations, *Philosophical Transactions of the Royal Society A: Mathematical, Physical, and Engineering Sciences*, 2021, **379**, 20200221, 10.1098/rsta.2020.0221

Groves AR, Ashton TE, **Darr JA**, High Throughput Synthesis and Screening of Oxygen Reduction Catalysts in the MTiO<sub>3</sub> (M = Ca, Sr, Ba) Perovskite Phase Diagram, *ACS Combinatorial Science*, 2020, **22**, 750-756, 10.1021/acscombsci.0c00094

Gurunatha KL, Sathasivam S, Li J, Portnoi M, **Parkin IP**, Papakonstantinou I, Combined Effect of Temperature Induced Strain and Oxygen Vacancy on Metal-Insulator Transition of VO<sub>2</sub> Colloidal Particles, *Advanced Functional Materials*, 2020, **30**, 2005311, 10.1002/adfm.202005311

Güsken NA, Lauri A, Li Y, Jacassi A, Matsui T, Doiron B, Bower R, **Regoutz A**, Mihai A, Petrov PK, Oulton RF, Cohen LF, Maier SA, IR hot carrier based photodetection in titanium nitride oxide thin film-Si junctions, *MRS Advances*, 2020, **5**, 1843-1850, 10.1557/adv.2020.129

Gutierrez SA, Marchello G, De Pace C, Ing G, Vazquez CL, Pilotto S, Werner F, Wilkinson N, **Gervasio FL**, **Ruiz-Perez L**, **Battaglia G**, Beyond Structure. Imaging Protein Dynamics at Physiological Temperatures, *Biophysical Journal*, 2021, **120**, 173A, 10.1016/j.bpj.2020.11.1219

Habib F, **Tocher DA**, Press NJ, **Carmalt CJ**, Structure determination of terpenes by the crystalline sponge method, *Microporous and Mesoporous Materials*, 2020, **308**, 110548, 10.1016/j.micromeso.2020.110548



**Hailes HC**, Subrizi F, Wang Y, Thair B, Mendez-Sanchez HD, Roddan R, Cardenas-Fernandez M, Siegrist J, Richter M, Andexer J, Ward J, Multienzyme one-pot cascades incorporating methyltransferases for the strategic diversification of tetrahydroisoquinoline alkaloids, *Angewandte Chemie International Edition*, 2021, **60**, 18673-18679, 10.1002/anie.202104476

Hall CL, Guo R, Potticary J, Cremeens ME, Warren SD, Andrusenko I, Gemmi M, **Zwijnenburg MA**, Sparkes HA, Pridmore NE, **Price SL**, Hall SR, Color differences highlight concomitant polymorphism of chalcones, *Crystal Growth & Design*, 2020, **20**, 6346-6355, 10.1021/acs.cgd.0c00285

Hartley P, Egdell RG, Zhang KHL, Hohmann MV, Piper LFJ, Morgan DJ, **Scanlon DO**, Williamson BAD, **Regoutz A**, Experimental and theoretical study of the electronic structures of lanthanide indium perovskites LnInO<sub>3</sub>, *The Journal of Physical Chemistry C*, 2021, **125**, 6387-6400, 10.1021/acs.jpcc.0c11592

Hasanli N, Scrimshire A, Bingham PA, **Palgrave RG**, Hayward MA, Structure and magnetism of the Rh<sup>4+</sup>-containing perovskite oxides La<sub>0.5</sub>Sr<sub>0.5</sub>Mn<sub>0.5</sub>Rh<sub>0.5</sub>O<sub>3</sub> and La<sub>0.5</sub>Sr<sub>0.5</sub>Fe<sub>0.5</sub>Rh<sub>0.5</sub>O<sub>3</sub>, *Dalton Transactions*, 2020, **49**, 11346-11353, 10.1039/d0dt02466j

Hasnain J, Jiang Y, Hou H, Yan J, Athanasopoulou L, **Forth J**, Ashby PD, Helms BA, Russell TP, Geissler PL, Spontaneous emulsification induced by nanoparticle surfactants, *The Journal of Chemical Physics*, 2020, **153**, 224705, 10.1063/5.0029016

Heath-Apostolopoulos I, Vargas-Ortiz D, Wilbraham L, Jelfs KE, **Zwijnenburg MA**, Using high-throughput virtual screening to explore the optoelectronic property space of organic dyes; finding diketopyrrolopyrrole dyes for dye-sensitized water splitting and solar cells, *Sustainable Energy & Fuels*, 2021, **5**, 704-719, 10.1039/d0se00985g

Heenan TMM, Vamvakeros A, Tan C, Finegan DP, Daemi SR, Jacques SDM, **Beale AM**, Di Michiel M, Brett DJL, Shearing PR, The detection of monoclinic zirconia and non-uniform 3d crystallographic strain in a re-oxidized Ni-YSZ solid oxide fuel cell anode, *Crystals*, 2020, **10**, 941, 10.3390/cryst10100941

Heo KJ, Jeong SB, Shin J, **Hwang GB**, Ko HS, Kim Y, Choi DY, Jung JH, Water-repellent TiO<sub>2</sub>-organic dye-based air filters for efficient visible-light-activated photochemical inactivation against bioaerosols, *Nano Letters*, 2020, **21**, 1576-1583, 10.1021/acs.nanolett.0c03173

Heritage K, Bryant B, Fenner LA, **Wills AS**, Aeppli G, Soh YA, Images of a first-order spin-reorientation phase transition in a metallic kagome ferromagnet, *Advanced Functional Materials*, 2020, **30**, 1909163, 10.1002/adfm.201909163

Higham MD, Mora-Fonz D, Sokol AA, **Woodley SM**, **Catlow CRA**, Morphology of Cu clusters supported on reconstructed polar ZnO (0001) and (000 $\bar{1}$ ) surfaces, *Journal of Materials Chemistry A*, 2020, **8**, 22840-22857, 10.1039/d0ta08351h

Hobson K, **Carmalt CJ**, **Bakewell C**, Aluminum amidinates: insights into alkyne hydroboration, *Inorganic Chemistry*, 2021, **60**, 10958-10969, 10.1021/acs.inorgchem.1c00619

Hobson K, **Carmalt CJ**, **Bakewell C**, Recent advances in low oxidation state aluminium chemistry, *Chemical Science*, 2020, **11**, 9028, 10.1039/d0sc90149k

Huang Y-T, Kavanagh SR, **Scanlon DO**, Walsh A, Hoye RLZ, Perovskite-inspired materials for photovoltaics and beyond-from design to devices, *Nanotechnology*, 2021, **32**, 132004, 10.1088/1361-6528/ac074b

Hudson JM, **Hele TJH**, Evans EW, Efficient light-emitting diodes from organic radicals with doublet emission, *Journal of Applied Physics*, 2021, **129**, 180901, 10.1063/5.0047636

Hutereau M, Banks PA, **Slater B**, Zeitler JA, Bond AD, Ruggiero MT, Resolving Anharmonic Lattice Dynamics in Molecular Crystals with X-Ray Diffraction and Terahertz Spectroscopy, *Physical Review Letters*, 2020, **125**, 103001, 10.1103/PhysRevLett.125.103001

**Hwang GB**, Wu G, Shin J, Panariello L, Sebastian V, Karu K, Allan E, Gavriilidis A, **Parkin IP**, Continuous single-phase synthesis of [Au<sub>25</sub>(Cys)<sub>18</sub>] nanoclusters and their photobactericidal enhancement, *ACS Applied Materials & Interfaces*, 2020, **12**, 49021-49029, 10.1021/acsami.0c07691

Ilmjärv S, Abdul F, Acosta-Gutiérrez S, Estarellas C, Galdadas I, Casimir M, Alessandrini M, **Gervasio FL**, Krause K-H, Concurrent mutations in RNA-dependent RNA polymerase and spike protein emerged as the epidemiologically most successful SARS-CoV-2 variant, *Scientific Reports*, 2021, **11**, 13705, 10.1038/s41598-021-91662-w

Imtiaz S, Amiinu IS, **Xu Y**, Kennedy T, **Blackman C**, Ryan KM, Progress and perspectives on alloying-type anode materials for advanced potassium-ion batteries, *Materials Today*, 2021, 10.1016/j.mattod.2021.02.008

Iqbal A, Kafizas A, Sotelo-Vazquez C, Wilson R, Ling M, Taylor A, **Blackman C**, Bevan K, **Parkin I**, Quesada-Cabrera R, Charge transport phenomena in heterojunction photocatalysts: the WO<sub>3</sub>/TiO<sub>2</sub> system as an archetypical model, *ACS Applied Materials and Interfaces*, 2021, **13**, 9781-9793, 10.1021/acsami.0c19692

Isaacs MA, Parlett CMA, Robinson N, Durndell LJ, Manayil JC, Beaumont SK, Jiang S, Hondow NS, Lamb AC, Jampaiah D, Johns ML, Wilson K, Lee AF, A spatially orthogonal hierarchically porous acid–base catalyst for cascade and antagonistic reactions, *Nature Catalysis*, 2020, **3**, 921-931, 10.1038/s41929-020-00549-y

Isakov I, Faber H, Mottram AD, Das S, Grell M, **Regoutz A**, Kilmurray R, McLachlan MA, Payne DJ, Anthopoulos TD, Quantum confinement and thickness-dependent electron transport in solution-processed In<sub>2</sub>O<sub>3</sub> transistors, *Advanced Electronic Materials*, 2020, **6**, 2000682, 10.1002/aelm.202000682

Islam MJ, Granollers Mesa M, Osatiashtiani A, Taylor MJ, Manayil JC, Parlett CMA, Isaacs MA, Kyriakou G, The effect of metal precursor on copper phase dispersion and nanoparticle formation for the catalytic transformations of furfural, *Applied Catalysis B: Environmental*, 2020, **273**, 119062, 10.1016/j.apcatb.2020.119062

Janowicz NJ, Li H, Heale FL, **Parkin IP**, Papakonstantinou I, Tiwari MK, **Carmalt CJ**, Fluorine-free transparent superhydrophobic nanocomposite coatings from mesoporous silica, *Langmuir*, 2020, **36**, 13426-13438, 10.1021/acs.langmuir.0c01767

Jaśkaniec S, Kavanagh SR, Coelho J, Ryan S, Hobbs C, Walsh A, **Scanlon DO**, Nicolosi V, Solvent engineered synthesis of layered SnO for high-performance anodes, *npj 2D Materials and Applications*, 2021, **5**, 27, 10.1038/s41699-021-00208-1

Jia S, Deng S, Qing Y, He G, Deng X, Luo S, Wu Y, Guo J, **Carmalt CJ**, Lu Y, **Parkin IP**, A coating-free superhydrophobic sensing material for full-range human motion and microliter droplet impact detection, *Chemical Engineering Journal*, 2021, **410**, 128418, 10.1016/j.cej.2021.128418

Jiao Y, Kang L, Berry-Gair J, McColi K, Li J, Dong H, Jiang H, Wang R, **Corà F**, Brett DJL, He G, **Parkin IP**, Enabling stable MnO<sub>2</sub> matrix for aqueous zinc-ion battery cathodes, *Journal of Materials Chemistry A*, 2020, **8**, 22075-22082, 10.1039/d0ta08638j

Johnson ID, Nolis G, Yin L, Yoo HD, Parajuli P, Mukherjee A, Andrews JL, Lopez M, Klie RF, Banerjee S, Ingram BJ, Lapidus S, Cabana J, **Darr JA**, Enhanced charge storage of nanometric ζ-V<sub>2</sub>O<sub>5</sub> in Mg electrolytes, *Nanoscale*, 2020, **12**, 22150-22160, 10.1039/d0nr05060a

Johnson ID, Stapleton N, Nolis G, Bauer D, Parajuli P, Yoo HD, Yin L, Ingram BJ, Klie RF, Lapidus S, **Darr JA**, Cabana J, Control of crystal size tailors the electrochemical performance of alpha-V<sub>2</sub>O<sub>5</sub> as a Mg<sup>2+</sup> intercalation host, *Nanoscale*, 2021, **13**, 10081-10091, 10.1039/d1nr03080a

Jones SF, Joshi H, Terry SJ, Burns JR, Aksimentiev A, Eggert US, **Howorka S**, Hydrophobic interactions between dna duplexes and synthetic and biological membranes, *Journal of the American Chemical Society*, 2021, **143**, 8305-8313, 10.1021/jacs.0c13235

Kabalan L, Kowalec I, **Catlow CRA**, Logsdaill AJ, A computational study of the properties of low- and high-index Pd, Cu and Zn surfaces, *Physical Chemistry Chemical Physics*, 2021, **23**, 14649-14661, 10.1039/d1cp01602d

Kalha C, Bichelmaier S, Fernando NK, Berens JV, Thakur PK, Lee TL, Gutiérrez Moreno JJ, Mohr S, Ratcliff LE, Reisinger M, Zechner J, Nelhiebel M, **Regoutz A**, Thermal and oxidation stability of Ti<sub>x</sub>W<sub>1-x</sub> diffusion barriers investigated by soft and hard X-ray photoelectron spectroscopy, *Journal of Applied Physics*, 2021, **129**, 195302, 10.1063/5.0048304

Kalha C, Fernando NK, Bhatt P, Johansson F, Linblad A, Rensmo H, Zendejas Mendina L, Lindblad R, Siol S, Jeurgens L, Cancellieri C, Rossnagel K, Medjanik K, Schoenhense G, Simon M, Gray A, Nemsak S, Lömker P, Schlueter C, **Regoutz A**, Hard X-ray photoelectron spectroscopy: a snapshot of the state-of-the-art in 2020, *Journal of Physics: Condensed Matter*, 2021, **33**, 233001, 10.1088/1361-648X/abeacd

Kamat K, Guo R, Reutzel-Edens SM, **Price SL**, Peters B, Diabat method for polymorph free energies: extension to molecular crystals, *The Journal of Chemical Physics*, 2020, **153**, 244105, 10.1063/5.0024727

Kang L, Wang B, Thetford A, Wu K, Danaie M, He Q, Gibson E, Sun L-D, Asakura H, **Catlow R**, Wang FR, Design, identification, and evolution of a surface ruthenium(ii/iii) single site for co activation, *Angewandte Chemie International Edition*, 2021, **60**, 1212-1219, 10.1002/anie.202008370

Karsten T, Middelkoop V, Matras D, Vamvakeros A, Poulston S, Grosjean N, Rollins B, Gallucci F, Godini HR, Jacques SDM, **Beale AM**, Repke J-U, Multi-scale studies of 3D printed Mn–Na–W/SiO<sub>2</sub> catalyst for oxidative coupling of methane, *Catalysts*, 2021, **11**, 290, 10.3390/catal11030290

Kavanagh SR, Walsh A, **Scanlon DO**, Rapid recombination by cadmium vacancies in CdTe, *ACS Energy Letters*, 2021, **6**, 1392-1398, 10.1021/acscenergylett.1c00380  
King AM, Bray C, Hall SCL, Bear JC, Bogart LK, Perrier S, **Davies G-L**, Exploring precision polymers to fine-tune magnetic resonance imaging properties of iron oxide nanoparticles, *Journal of Colloid and Interface Science*, 2020, **579**, 401-411, 10.1016/j.jcis.2020.06.036

Kocere A, Resseguier J, Wohlmann J, Skjeldal FM, Khan S, Speth M, Dal NJK, Ng MYW, Alonso-Rodriguez N, Scarpa E, Rizzello L, **Battaglia G**, Griffiths G, Fenaroli F, Real-time imaging of polymersome nanoparticles in zebrafish embryos engrafted with melanoma cancer cells: Localization, toxicity and treatment analysis, *EBioMedicine*, 2020, **58**, 102902, 10.1016/j.ebiom.2020.102902

Kumar S, Hassan I, Regue M, Gonzalez-Carrero S, Rattner E, Isaacs MA, Eslava S, Mechanochemically synthesized Pb-free halide perovskite-based Cs<sub>2</sub>AgBiBr<sub>6</sub>–Cu–RGO nanocomposite for photocatalytic CO<sub>2</sub> reduction, *Journal of Materials Chemistry A*, 2021, **9**, 12179-12187, 10.1039/d1ta01281a

Laassiri S, Zeinalipour-Yazdi CD, Bion N, **Catlow CRA**, Hargreaves JSJ, Combination of theoretical and *in situ* experimental investigations of the role of lithium dopant in manganese nitride: a two-stage reagent for ammonia synthesis, *Faraday Discussions*, 2021, **229**, 281-296, 10.1039/c9fd00131j

Lais T, Lukashuk L, van de Water L, Hyde TI, Aramini M, **Sankar G**, Elucidation of copper environment in a Cu–Cr–Fe oxide catalyst through *in situ* high-resolution XANES investigation, *Physical Chemistry Chemical Physics*, 2021, **23**, 5888-5896, 10.1039/d0cp06468h

Lanphere C, Arnott PM, Jones SF, Korlova K, **Howorka S**, A biomimetic DNA-based membrane gate for protein-controlled transport of cytotoxic drugs, *Angewandte Chemie International Edition*, 2020, **60**, 1903-1908, 10.1002/anie.202011583

Lanphere C, Offenbartl-Stiegert D, Dorey A, Pugh G, Georgiou E, Xing Y, Burns JR, **Howorka S**, Design, assembly, and characterization of membrane-spanning DNA nanopores, *Nature Protocols*, 2021, **16**, 86-130, 10.1038/s41596-020-0331-7

Leach AS, Hack J, Amboage M, Diaz-Moreno S, Huang H, Cullen PL, Wilding M, Magliocca E, Miller T, Howard C, Brett D, Shearing P, **McMillan PF**, Russell AE, Jervis R, A novel fuel cell design for operando energy-dispersive X-ray absorption measurements, *Journal of Physics: Condensed Matter*, 2021, **33**, 314002, 10.1088/1361-648X/ac0476

Lehr A, Gomez Rodriguez S, Parkes MA, **Worth G**, The role of vibronic coupling in the electronic spectroscopy of maleimide: a multi-mode and multi-state quantum dynamics study, *Physical Chemistry Chemical Physics*, 2020, **22**, 25272-25283, 10.1039/d0cp04514d

Leung CLA, Elizarova I, Isaacs M, Marathe S, Saiz E, Lee PD, Enhanced near-infrared absorption for laser powder bed fusion using reduced graphene oxide, *Applied Materials Today*, 2021, **23**, 101009, 10.1016/j.apmt.2021.101009

Lezcano-Gonzalez I, Campbell E, Hoffman AEJ, Bocus M, Sazanovich IV, Towrie M, Agote-Aran M, Gibson EK, Greenaway A, De Wispelaere K, Van Speybroeck V, **Beale AM**, Insight into the effects of confined hydrocarbon species on the lifetime of methanol conversion catalysts, *Nature Materials*, 2020, **19**, 1081-1087, 10.1038/s41563-020-0800-y

Li Q, Wang H, Tang X, Zhou M, Zhao H, **Xu Y**, Xiao W, Lei Y, Electrical conductivity adjustment for interface capacitive-like storage in sodium-ion battery, *Advanced Functional Materials*, 2021, **31**, 2101081, 10.1002/adfm.202101081

Li Z, Kavanagh SR, Napari M, **Palgrave R**, Abdi-Jalebi M, Andaji-Garmaroudi Z, Davies D, Laitinen M, Julin J, Isaacs MA, Friend R, **Scanlon DO**, Walsh A, Hoye RLZ, bandgap lowering in mixed alloys of Cs<sub>2</sub>Ag(Sb<sub>x</sub>Bi<sub>1-x</sub>)Br<sub>6</sub> double perovskite thin films, *Journal of Materials Chemistry A*, 2020, **8**, 21780-21788, 10.1039/d0ta07145e

Limburn GJ, Stephens MJP, Williamson BAD, Iborra-Torres A, **Scanlon DO**, Hyett G, Photocatalytic, structural and optical properties of mixed anion solid solutions Ba<sub>3</sub>Sc<sub>2-x</sub>In<sub>x</sub>O<sub>5</sub>Cu<sub>2</sub>S<sub>2</sub> and Ba<sub>3</sub>In<sub>2</sub>O<sub>5</sub>Cu<sub>2</sub>S<sub>2-y</sub>Se<sub>y</sub>, *Journal of Materials Chemistry A*, 2020, **8**, 19887-19897, 10.1039/d0ta06629j

Liu B, Xu S, Zhang M, Li X, Decarolis D, Liu Y, Wang Y, Gibson EK, **Catlow CRA**, Yan K, Electrochemical upgrading of biomass-derived 5-hydroxymethylfurfural and furfural over oxygen vacancy-rich NiCoMn-layered double hydroxides nanosheets, *Green Chemistry*, 2021, **23**, 4034-4043, 10.1039/d1gc00901j



Liu M, Apriceno A, Sipin M, Scarpa E, Rodriguez-Arco L, Poma A, Marchello G, **Battaglia G**, Angioletti-Uberti S, Combinatorial entropy behaviour leads to range selective binding in ligand-receptor interactions, *Nature Communications*, 2020, **11**, 4836, 10.1038/s41467-020-18603-5

Liu M, Konstantinova M, **Negahdar L**, McGregor J, The role of Zn in the sustainable one-pot synthesis of dimethyl carbonate from carbon dioxide, methanol and propylene oxide, *Chemical Engineering Science*, 2020, **231**, 116267, 10.1016/j.ces.2020.116267

Liu Q, Tian S, Zhao X, **Sankar G**, An enhanced fluorescent ZIF-8 film by capturing guest molecules for light-emitting applications, *Journal of Materials Chemistry C*, 2021, **9**, 5819-5826, 10.1039/d1tc00457c

Liu Y, Niu Z, Dai G, Chen Y, Li H, Huang L, Zhang X, **Xu Y**, Zhao Y, Phenothiazine-based copolymer with redox functional backbones for organic battery cathode materials, *Materials Today Energy*, 2021, 100812, 10.1016/j.mtener.2021.100812

Lo Faro MJ, Ruello G, Leonardi AA, Morganti D, Irrera A, Priolo F, Gigan S, **Volpe G**, Fazio B, Visualization of directional beaming of weakly localized raman from a random network of silicon nanowires, *Advanced Science*, 2021, 2100139, 10.1002/adv.202100139

Lu Z, Zhu B, Shires BWB, **Scanlon DO**, Pickard CJ, Ab initio random structure searching for battery cathode materials, *The Journal of Chemical Physics*, 2021, **154**, 174111, 10.1063/5.0049309

Lunn RDJ, **Tocher DA**, Sidebottom PJ, Montgomery MG, Keates AC, **Carmalt CJ**, Encapsulation of aromatic compounds and a non-aromatic herbicide into a gadolinium-based metal–organic framework via the crystalline sponge method, *Crystal Growth & Design*, 2020, **20**, 7238-7245, 10.1021/acs.cgd.0c00901

Lunn RDJ, **Tocher DA**, Sidebottom PJ, Montgomery MG, Keates AC, **Carmalt CJ**, Applying the crystalline sponge method to agrochemicals: obtaining x-ray structures of the fungicide Metalaxyl-M and herbicide S-Metolachlor, *Crystal Growth & Design*, 2021, **21**, 3024-3036, 10.1021/acs.cgd.1c00196

Lv X, Wang W, **Clancy AJ**, Yu H, High-Speed, Heavy-Load, and Direction-Controllable Photothermal Pneumatic Floating Robot, *ACS Applied Materials and Interfaces*, 2021, **13**, 23030-23037, 10.1021/acsami.1c05827

M Leite D, Matias D, **Battaglia G**, The role of bar proteins and the glycocalyx in brain endothelium transcytosis, *Cells*, 2020, **9**, 2685, 10.3390/cells9122685

**Abraham MH**, Acree Jr. WE, Liu X, Descriptors for adamantane and some of its derivatives, *Journal of Molecular Liquids*, 2021, **325**, 114894, 10.1016/j.molliq.2020.114894

Maitra A, Evangelopoulos D, Chrzastek A, Martin LT, Hanrath A, Chapman E, **Hailes HC**, Lipman M, McHugh TD, Waddell SJ, Bhakta S, Carprofen elicits pleiotropic mechanisms of bactericidal action with the potential to reverse antimicrobial drug resistance in tuberculosis, *Journal of Antimicrobial Chemotherapy*, 2020, **75**, 3194-3201, 10.1093/jac/dkaa307

Maitra A, Nukala S, Dickman R, Martin LT, Munshi T, Gupta A, Shepherd AJ, Arnvig KB, **Tabor AB**, Keep NH, Bhakta S, Characterization of the MurT/GatD complex in *Mycobacterium tuberculosis* towards validating a novel anti-tubercular drug target, *JAC-Antimicrobial Resistance*, 2021, **3**, dlab028, 10.1093/jacamr/dlab028

Malinowski R, **Parkin IP**, **Volpe G**, Nonmonotonic contactless manipulation of binary droplets via sensing of localized vapor sources on pristine substrates, *Science Advances*, 2020, **6**, 2375-2548, 10.1126/sciadv.aba3636

Manning JRH, Brambila C, Patwardhan SV, Unified mechanistic interpretation of amine-assisted silica synthesis methods to enable design of more complex materials, *Molecular Systems Design & Engineering*, 2021, **6**, 170-196, 10.1039/d0me00131g

Manning JRH, Walkley B, Provis JL, Patwardhan SV, Mimicking biosintering: the identification of highly condensed surfaces in bioinspired silica materials, *Langmuir*, 2021, **37**, 561-568, 10.1021/acs.langmuir.0c03261

Mant B, Franz J, Wester R, Gianturco FA, Beyond the helium buffer: <sup>12</sup>C<sub>2</sub><sup>-</sup> rotational cooling in cold traps with H<sub>2</sub> as a partner gas: interaction forces and quantum dynamics, *Molecular Physics*, 2021, 10.1080/00268976.2021.1938267

Marcolan C, Glaser M, Twyman F, **Sander K**, Awais R, **Arstad E**, A generic gc protocol for the residual solvent analysis of PET radiopharmaceuticals, *European Journal of Nuclear Medicine and Molecula Imaging*, 2020, **47**, S683

Marin-Beloqui JM, Toolan DTW, Panjwani NA, Limbu S, Kim JS, **Clarke TM**, Triplet-charge annihilation in a small molecule donor: acceptor blend as a major loss mechanism in organic photovoltaics, *Advanced Energy Materials*, 2021, **11**, 2100539, 10.1002/aenm.202100539

Matam SK, Moffat C, Hellier P, Bowker M, Silverwood IP, **Catlow CRA**, David Jackson S, Craswell J, Wells PP, Parker SF, Gibson EK, Investigation of MoO<sub>x</sub>/Al<sub>2</sub>O<sub>3</sub> under cyclic operation for oxidative and non-oxidative dehydrogenation of propane, *Catalysts*, 2020, **10**, 1-13, 10.3390/catal10121370

Matras D, Vamvakeros A, Jacques SDM, di Michiel M, Middelkoop V, Ismagilov IZ, Matus EV, Kuznetsov VV, Cernik RJ, **Beale AM**, Multi-length scale 5D diffraction imaging of Ni-Pd/CeO<sub>2</sub>-ZrO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> catalyst during partial oxidation of methane, *Journal of Materials Chemistry A*, 2021, **9**, 11331-11346, 10.1039/d1ta01464a

McColl K, **Corà F**, Fast lithium-ion conductivity in the ‘empty-perovskite’ n = 2 Ruddlesden–Popper-type oxysulphide Y<sub>2</sub>Ti<sub>2</sub>S<sub>2</sub>O<sub>s</sub>, *Journal of Materials Chemistry A*, 2021, **9**, 7068-7084, 10.1039/d0ta11358a

McConnell AJ, **Haynes CJE**, Caltagirone C, Hiscock JR, Supramolecular Chemistry: Young Talents and their Mentors, *ChemPlusChem*, 2020, **85**, 2544-2545, 10.1002/cplu.202000668

McCullough JWS, Richardson RA, Patronis A, Halver R, Marshall R, Ruefenacht M, Wylie BJN, Odaker T, Wiedemann M, Lloyd B, Neufeld E, Sutmann G, Skjellum A, Kranzlmüller D, **Coveney PV**, Towards blood flow in the virtual human: Efficient self-coupling of HemeLB, *Interface Focus*, 2021, **11**, 20190119, 10.1098/rsfs.2019.0119

McGhee JR, Goulas A, Southee DJ, Sagu JS, Engstrøm DS, Wang J, Hutt DA, Evans PSA, Zhou Z, Wijayantha KGU, Conway P, **Carmalt CJ**, Indium tin oxide nanowires manufactured via printing and laser irradiation, *Applied Materials Today*, 2020, **21**, 100835, 10.1016/j.apmt.2020.100835

Mears KL, Stennett CR, Taskinen EK, **Knapp CE**, **Carmalt CJ**, Tuononen HM, Power PP, Molecular Complexes Featuring Unsupported Dispersion-Enhanced Aluminum–Copper and Gallium–Copper Bonds, *Journal of the American Chemical Society*, 2020, **142**, 19874-19878, 10.1021/jacs.0c10099

Mewes L, **Ingle RA**, Al Haddad A, Chergui M, Broadband visible two-dimensional spectroscopy of molecular dyes, *The Journal of Chemical Physics*, 2021, **155**, 034201, 10.1063/5.0053554

Mewes L, Wang M, **Ingle RA**, Borjesson K, Chergui M, Energy relaxation pathways between light-matter states revealed by coherent two-dimensional spectroscopy, *Communications Physics*, 2020, **3**, 157, 10.1038/s42005-020-00424-z

Minova IB, Matam SK, Greenaway A, **Catlow CRA**, Frogley MD, Cinque G, Wright PA, Howe RF, Effects of crystal size on methanol to hydrocarbon conversion over single crystals of ZSM-5 studied by synchrotron infrared microspectroscopy, *Physical Chemistry Chemical Physics*, 2020, **22**, 18849-18859, 10.1039/d0cp00704h

Mitchell CE, Santos-Carballal D, **Beale AM**, Jones W, Morgan DJ, Sankar M, de Leeuw NH, The role of surface oxidation and Fe-Ni synergy in Fe-Ni-S catalysts for CO<sub>2</sub> hydrogenation, *Faraday Discussions*, 2021, **230**, 30-51, 10.1039/d0fd00137f

Mitchell CE, Terranova U, **Beale AM**, Jones W, Morgan DJ, Sankar M, de Leeuw NH, A surface oxidised Fe-S catalyst for the liquid phase hydrogenation of CO<sub>2</sub>, *Catalysis Science and Technology*, 2021, **11**, 779-784, 10.1039/d0cy01779e

Mitscha-Baude G, Stadlbauer B, **Howorka S**, Heitzinger C, Protein transport through nanopores illuminated by long-time-scale simulations, *ACS Nano*, 2021, **15**, 9900-9912, 10.1021/acsnano.1c01078

Morais M, Nunes JPM, Karu K, Forte N, Benni I, Smith MEB, **Caddick S**, **Chudasama V**, **Baker JR**, Optimisation of the dibromomaleimide (DBM) platform for native antibody conjugation by accelerated post-conjugation hydrolysis , *Organic & Biomolecular Chemistry*, 2021, **19**, 3024, 10.1039/d1ob90035h

Morozov IG, Belousova OV, Sathasivam S, **Parkin IP**, Kuznetsov MV, Some peculiarities of room-temperature ferromagnetism in ensembles of mixed-phase TiN<sub>x</sub>TiO<sub>y</sub> nanoparticles, *Materials Research Bulletin*, 2021, **134**, 111092, 10.1016/j.materresbull.2020.111092

Mortensen M, Huckvale R, Pandurangan AP, **Baker JR**, Smart TG, Optopharmacology reveals a differential contribution of native GABAA receptors to dendritic and somatic inhibition using azogabazine, *Neuropharmacology*, 2020, **176**, 108135, 10.1016/j.neuropharm.2020.108135

Moss B, Le H, Corby S, Morita K, Selim S, Sotelo-Vazquez C, Chen Y, Borthwick A, Wilson A, **Blackman C**, Durrant JR, Walsh A, Kafizas A, Anisotropic electron transport limits performance of Bi<sub>2</sub>WO<sub>6</sub> photoanodes, *The Journal of Physical Chemistry C*, 2020, **124**, 18859-18867, 10.1021/acs.jpcc.0c03539

Moss B, Wang Q, Butler KT, Grau-Crespo R, Selim S, **Regoutz A**, Hisatomi T, Godin R, Payne DJ, Kafizas A, Domen K, Steier L, Durrant JR, Linking in situ charge accumulation to electronic structure in doped SrTiO<sub>3</sub> reveals design principles for hydrogen-evolving photocatalysts, *Nature Materials*, 2021, **20**, 511-517, 10.1038/s41563-020-00868-2

Nadeem IM, Hargreaves L, Harrison GT, Idriss H, Shluger AL, **Thornton G**, Carboxylate adsorption on rutile tio2(100): role of coulomb repulsion, relaxation, and steric hindrance, *The Journal of Physical Chemistry C*, 2021, **125**, 13770-13779, 10.1021/acs.jpcc.1c00892

Nasir JA, Rehman ZU, Shah SNA, Khan A, Butler IS, **Catlow CRA**, Recent developments and perspectives in CdS-based photocatalysts for water splitting, *Journal of Materials Chemistry A*, 2020, **8**, 20752-20780, 10.1039/d0ta05834c

Nastase SAF, **Catlow CRA**, Logsdaile AJ, QM/MM study of the stability of dimethyl ether in zeolites H-ZSM-5 and H-Y, *Physical Chemistry Chemical Physics*, 2020, **23**, 2088-2096, 10.1039/d0cp05392a

Nastase SAF, Cnudde P, Vanduyfhuys L, De Wispelaere K, Van Speybroeck V, **Catlow CRA**, Logsdaile AJ, Mechanistic insight into the framework methylation of h-zsm-5 for varying methanol loadings and Si/Al ratios using first-principles molecular dynamics simulations, *ACS Catalysis*, 2020, **10**, 8904-8915, 10.1021/acscatal.0c01454

Nayak P, Xie R-C, **Palgrave RG**, Compton RG, Electro-oxidation of titanium carbide nanoparticles in aqueous acid creates TiC@TiO<sub>2</sub> core-shell structures, *ChemElectroChem*, 2021, **8**, 911-917, 10.1002/celc.202001498

Negahdar L, Xi X, Zeng F, Winkelman JGM, Heeres HJ, Palkovits R, CO hydrogenation over K-Co-MoS<sub>x</sub> catalyst to mixed alcohols: A kinetic analysis, *International Journal of Chemical Kinetics*, 2020, **53**, 419-427, 10.1002/kin.21453

Németh P, McColl K, Garvie LAJ, **Salzmänn CG**, Murri M, **McMillan PF**, Complex nanostructures in diamond, *Nature Materials*, 2020, **19**, 1126-1131, 10.1038/s41563-020-0759-8

Newgas SA, Jeffries JWE, Moody TS, Ward JM, **Hailes HC**, Discovery of New Carbonyl Reductases Using Functional Metagenomics and Applications in Biocatalysis, *Advanced Synthesis & Catalysis*, 2021, **363**, 3044-3052, 10.1002/adsc.202100199

Noble Jesus C, Evans R, Forth J, Estarellas C, **Gervasio FL**, **Battaglia G**, Amphiphilic histidine-based oligopeptides exhibit pH-reversible fibril formation, *ACS Macro Letters*, 2021, **10**, 984-989, 10.1021/acsmacrolett.1c00142

Olivucci M, Tran T, **Worth GA**, Robb MA, Unlocking the double bond in protonated schiff bases by coherent superposition of S1 and S2, *The Journal of Physical Chemistry Letters*, 2021, **12**, 5639-5643, 10.1021/acs.jpcclett.1c01379

Omori N, Candéo A, Mosca S, Lezcano-Gonzalez I, Robinson IK, Li L, Greenaway AG, Collier P, **Beale AM**, Multimodal imaging of autofluorescent sites reveals varied chemical speciation in SSZ-13 crystals, *Angewandte Chemie International Edition*, 2020, **60**, 5125-5131, 10.1002/anie.202015016

Panchal M, Callison J, Skukauskas V, Gianolio D, Cibir G, York APE, Schuster ME, Hyde TI, Collier P, **Catlow CRA**, Gibson EK, Operando XAFS investigation on the effect of ash deposition on three-way catalyst used in gasoline particulate filters and the effect of the manufacturing process on the catalytic activity, *Journal of Physics: Condensed Matter*, 2021, **33**, 284001, 10.1088/1361-648X/abfe16

Papamatthaiou S, Zupancic U, Kalha C, **Regoutz A**, Estrela P, Moschou D, Ultra stable, inkjet-printed pseudo reference electrodes for lab-on-chip integrated electrochemical biosensors, *Scientific Reports*, 2020, **10**, 17152, 10.1038/s41598-020-74340-1

Patel AM, Henley A, Parkes MA, Assmann M, **Worth GA**, **Anderson JC**, **Fielding HH**, Shining light on the electronic structure and relaxation dynamics of the isolated oxyluciferin anion, *Physical Chemistry Chemical Physics*, 2020, **22**, 19022-19032, 10.1039/d0cp03276j

Pathak S, Ibele LM, Boll R, Callegari C, Demidovich A, Erk B, Feifel R, Forbes R, Di Fraia M, Giannessi L, Hansen CS, Holland DMP, **Ingle RA**, Mason R, Plekan O, Prince KC, Rouzée A, Squibb RJ, Tross J, Ashfold MNR, Curchod BFE, Rolles D, Tracking the ultraviolet-induced photochemistry of thiophenone during and after ultrafast ring opening, *Nature Chemistry*, 2020, **12**, 795-800, 10.1038/s41557-020-0507-3

Patir A, Hwang GB, Lourenco C, Nair SP, **Carmalt CJ**, **Parkin IP**, Crystal Violet-Impregnated Slippery Surface to Prevent Bacterial Contamination of Surfaces, *ACS Applied Materials & Interfaces*, 2021, **13**, 5478-5485, 10.1021/acsami.0c17915

Perona Martínez F, Nusantara AC, Chipaux M, Padamati SK, Schirhagl R, Nanodiamond relaxometry-based detection of free-radical species when produced in chemical reactions in biologically relevant conditions, *ACS Sensors*, 2020, **5**, 3862-3869, 10.1021/acssensors.0c01037

Pink DL, Foglia F, Barlow DJ, Lawrence MJ, Lorenz CD, the impact of lipid digestion on the dynamic and structural properties of micelles, *Small*, 2021, **17**, 2004761, 10.1002/smll.202004761



Pira A, Scorciapino MA, Bodrenko IV, Bosin A, Acosta-Gutiérrez S, Ceccarelli M, Permeation of  $\beta$ -lactamase inhibitors through the general porins of gram-negative bacteria, *Molecules*, 2020, **25**, 5747, 10.3390/molecules25235747

Popadić D, Mhaindarkar D, Dang Thai MHN, **Hailes HC**, Mordhorst S, Andexer JN, A bicyclic S-adenosylmethionine regeneration system applicable with different nucleosides or nucleotides as cofactor building blocks, *RSC Chemical Biology*, 2021, **2**, 883-891, 10.1039/d1cb00033k  
Portnoi M, Haigh PA, Macdonald TJ, Ambroz F, **Parkin IP**, Darwazeh I, Papakonstantinou I, Bandwidth limits of luminescent solar concentrators as detectors in free-space optical communication systems, *Light Science & Applications*, 2021, **10**, 3, 10.1038/s41377-020-00444-y

**Powner M**, Colville B, Selective prebiotic synthesis of  $\alpha$ -Threofuranosyl Cytidine by photochemical anomerization, *Angewandte Chemie International Edition*, 2021, **60**, 10526-10530, 10.1002/anie.202101376

**Powner M**, Islam S, Foden C, Fernandez Garcia CA, Maugeri L, **Sheppard T**, Prebiotic synthesis of cysteine peptides that catalyze peptide ligation in neutral water, *Science*, 2020, **370**, 865-869, 10.1126/science.abd5680

Prentice A, **Zwijnenburg M**, Hydrogen evolution by polymer photocatalysts; a possible photocatalytic cycle, *Sustainable Energy & Fuels*, 2021, **5**, 2622-2632, 10.1039/d1se00059d

Prentice AW, Wildman J, Galbraith I, Paterson MJ, Properties of conjugated materials from quantum chemistry coupled to molecular dynamics generated ensembles, *The Journal of Physical Chemistry A*, 2020, **124**, 10667-10677, 10.1021/acs.jpca.0c07213  
Prentice AW, **Zwijnenburg MA**, The role of computational chemistry in discovering and understanding organic photocatalysts for renewable fuel synthesis, *Advanced Energy Materials*, 2021, 2100709, 10.1002/aenm.202100709

**Price SD**, Armenta Butt S, Bond-forming and electron-transfer reactivity between Ar2+ and N2, *Physical Chemistry Chemical Physics*, 2021, **23**, 11287-11299, 10.1039/D1CP00918D

Qiu C, Odarchenko Y, Meng Q, Cong P, Schoen MAW, Kleibert A, Forrest T, **Beale AM**, Direct observation of the evolving metal–support interaction of individual cobalt nanoparticles at the titania and silica interface, *Chemical Science*, 2020, **11**, 13060-13070, 10.1039/d0sc03113e

Quesada-Cabrera R, **Parkin IP**, Qualitative approaches towards useful photocatalytic materials, *Frontiers in Chemistry*, 2020, **8**, 817, 10.3389/fchem.2020.00817

Quesne MG, **Catlow CRA**, de Leeuw NH, How bulk and surface properties of Ti4SiC3, V4SiC3, Nb4SiC3 and Zr4SiC3 tune reactivity: a computational study, *Faraday Discussions*, 2021, **230**, 87-99, 10.1039/d1fd00004g

Rahim W, Cheng A, Lyu C, Shi T, Wang Z, **Scanlon D**, **Palgrave R**, Geometric analysis and formability of the cubic A2BX6 vacancy-ordered double perovskite structure, *Chemistry of Materials*, 2020, **32**, 9573-9583, 10.1021/acs.chemmater.0c02806

**Regoutz A**, Swolinska M, Fernando NK, Ratcliff LE, A combined density functional theory and X-ray photoelectron spectroscopy study of the aromatic amino acids, *Electronic Structure*, 2020, **2**, 044005, 10.1088/2516-1075/abd63c

Richards DA, Thomas MR, Szijj PA, Foote J, Chen Y, Nogueira JCF, **Chudasama V**, Stevens MM, Employing defined bioconjugates to generate chemically functionalised gold nanoparticles for *in vitro* diagnostic applications, *Nanoscale*, 2021, 10.1039/d1nr02584h

**Rivera M**, Stojanović L, Crespo-Otero R, Role of Conical Intersections on the Efficiency of Fluorescent Organic Molecular Crystals, *The Journal of Physical Chemistry A*, 2021, **125**, 1012-1024, 10.1021/acs.jpca.0c11072

Roddan R, Sula A, Méndez-Sánchez D, Subrizi F, Lichman BR, Broomfield J, Richter M, Andexer JN, Ward JM, Keep NH, **Hailes HC**, Single step syntheses of (1S)-aryl-tetrahydroisoquinolines by norcoclaurine synthases, *Communications Chemistry*, 2020, **3**, 170, 10.1038/s42004-020-00416-8

Rood S, Pastor-Algaba O, Tosca-Princep A, Pinho B, Isaacs M, Torrente-Murciano L, Eslava S, Synergistic Effect of Simultaneous Doping of Ceria Nanorods with Cu and Cr on CO Oxidation and NO Reduction, *Chemistry – A European Journal*, 2021, **27**, 2165-2174, 10.1002/chem.202004623

Roos G, Oláh J, **Ingle R**, Kobayashi R, Feldt M, Online conferences – towards a new (virtual) reality, *Computational and Theoretical Chemistry*, 2020, **1189**, 112975, 10.1016/j.comptc.2020.112975

Ruiz-Gonzalez A, **Clancy AJ**, Choy K-L, Rapid detection of free and bound toxins using molecularly imprinted silica/graphene oxide hybrids, *Chemical Communications*, 2021, **57**, 4043-4046, 10.1039/d1cc00572c

Ryan HP, **Haynes CJE**, Smith A, Grommet AB, Nitschke JR, Guest Encapsulation within Surface-Adsorbed Self-Assembled Cages, *Advanced Materials*, 2020, **33**, e2004192, 10.1002/adma.202004192

Soriano-Meseguer S, Fuguet E, **Abraham MH**, Port A, Roses M, Linear free energy relationships for the retention of partially ionized acid-base compounds in reversed-phase liquid chromatography, *Journal of Chromatography A*, 2020, **1635**, 461720, 10.1016/j.chroma.2020.461720

Wang S, Liu K, Zhang A, Dai J, Gupta A, Zhu S, Eddula S, Jiang C, Acree Jr. WE, **Abraham MH**, Solubility of 4-methyl-3-nitrobenzoic acid in organic mono-solvents: calculation of Abraham model solute descriptors, *Physics and Chemistry of Liquids*, 2020, **58**, 782-791, 10.1080/00319104.2019.1660982

Sadraeian M, Bahou C, da Cruz EF, Janini LMR, Diaz RS, Boyle RW, **Chudasama V**, Guimarães FEG, Photoimmunotherapy using cationic and anionic photosensitizer-antibody conjugates against HIV env-expressing cells, *International Journal of Molecular Sciences*, 2020, **21**, 9151, 10.3390/ijms21239151

Sadraeian M, da Cruz EF, Boyle RW, Bahou C, **Chudasama V**, Janini LMR, Diaz RS, Guimarães FEG, Photoinduced photosensitizer-antibody conjugates kill HIV env-expressing cells, also inactivating HIV, *ACS Omega*, 2021, **6**, 16524-16534, 10.1021/acsomega.1c01721

**Salzmann CG**, Loveday JS, Rosu-Finsen A, Bull CL, Structure and nature of ice XIX, *Nature Communications*, 2021, **12**, 3162, 10.1038/s41467-021-23399-z

**Salzmann CG**, Rosu-Finsen A, Sharif Z, Radaelli PG, Finney JL, Detailed crystallographic analysis of the ice V to ice XIII hydrogen-ordering phase transition, *The Journal of Chemical Physics*, 2021, **154**, 134504, 10.1063/5.0045443

**Salzmann CG**, Rosu-Finsen A, The crystallography of Pluto, *International Union of Crystallography*, 2020, **7**, 782-783, 10.1107/s205225252001163x

**Sander K**, Gendron T, Cybulska KA, Sirindil F, Zhou J, Kalber TL, Lythgoe MF, Kurzawinski TR, Brown MJ, Williams B, Årstad E, Development of [<sup>18</sup>F]AldoView as the first highly selective aldosterone synthase PET tracer for imaging of primary hyperaldosteronism, *Journal of Medicinal Chemistry*, 2021, **64**, 9321-9329, 10.1021/acs.jmedchem.1c00539

Santos M, O’Sullivan B, Müller S, Bunescu A, Baganz F, Marques MPC, **Hailes H**, Szita N, Wohlgemuth R, Chemoenzymatic microfluidic cascade reaction: Coupling of a diels-alder reaction with a transketolase-catalyzed reaction, *MicroTAS 2020 - 24th International Conference on Miniaturized Systems for Chemistry and Life Sciences*, 2020, 693-694

Sarkar C, Paul R, Shit SC, Quang TT, Koley P, Rao BS, **Beale AM**, Pao C-W, Banerjee A, Mondal J, Navigating copper-atom-pair structural effect inside a porous organic polymer cavity for selective hydrogenation of biomass-derived 5-Hydroxymethylfurfural, *ACS Sustainable Chemistry & Engineering*, 2021, **9**, 2136-2151, 10.1021/acssuschemeng.0c07594

Sarma PJ, Dowerah D, Gour NK, Logsdaill AJ, **Catlow CRA**, Deka RC, Tuning the transition barrier of H2 dissociation in the hydrogenation of CO2 to formic acid on Ti-doped Sn2Ox clusters, *Physical Chemistry Chemical Physics*, 2021, **23**, 204-210, 10.1039/d0cp04472e

Sayer JR, Wallden K, Koss H, Allan H, Daviter T, Gane PJ, Waksman G, **Tabor AB**, Design, synthesis, and evaluation of peptide-imidazo[1,2-a]pyrazine bioconjugates as potential bivalent inhibitors of the VirB11 ATPase HP0525, *Journal of Peptide Science*, 2021, e3353, 10.1002/psc.3353

Seavill PW, **Wilden JD**, The preparation and applications of amides using electrosynthesis, *Green Chemistry*, 2020, **22**, 7737-7759, 10.1039/d0gc02976a

Sehmi SK, Lourenco C, Alkhuder K, Pike SD, Noimark S, Williams CK, Shaffer MSP, **Parkin IP**, MacRobert AJ, Allan E, Antibacterial surfaces with activity against antimicrobial resistant bacterial pathogens and endospores, *ACS Infectious Diseases*, 2020, **6**, 939-946, 10.1021/acsinfecdis.9b00279

Shaikh J, Congrave DG, Forster A, Minotto A, Cacialli F, **Hele TJH**, Penfold TJ, Bronstein H, **Clarke TM**, Intrinsic photogeneration of long-lived charges in a donor-orthogonal acceptor conjugated polymer, *Chemical Science*, 2021, **12**, 8265-8177, 10.1039/d1sc00919b

Shan F, Panariello L, Wu G, Gavriilidis A, **Fielding HH**, **Parkin IP**, A study of the interaction of cationic dyes with gold nanostructures, *RSC Advances*, 2021, **11**, 17694-17703, 10.1039/d1ra03459f

Sharif Z, Shephard JJ, **Slater B**, Bull CL, Hart M, **Salzmann CG**, Effect of ammonium fluoride doping on the ice III to ice IX phase transition, *The Journal of Chemical Physics*, 2021, **154**, 114502, 10.1063/5.0032485

Sharma A, Singh S, Song X, Rosas Villalva D, Throughton J, Corzo D, Toppare L, Gunbas G, **Schroeder BC**, Baran D, A Nonionic Alcohol Soluble Polymer Cathode Interlayer Enables Efficient Organic and Perovskite Solar Cells, *Chemistry of Materials*, 2021, 10.1021/acs.chemmater.1c01430

Shivhare A, Hunns JA, Durnell LJ, Parlett CMA, Isaacs MA, Lee AF, Wilson K, Metal–Acid Synergy: Hydrodeoxygenation of Anisole over Pt/Al-SBA-15, *ChemSusChem*, 2020, **13**, 4775, 10.1002/cssc.202002011

**Simoncelli S**, Griffié J, Williamson DJ, Bibby J, Bray C, Zamoyka R, Cope AP, Owen DM, Multi-color molecular visualization of signaling proteins reveals how C-terminal Src kinase nanoclusters regulate T cell receptor activation, *Cell Press*, 2020, **33**, 108523, 10.1016/j.celrep.2020.108523

Sola-Barrado B, M. Leite D, Scarpa E, Duro-Castano A, **Battaglia G**, Combinatorial intracellular delivery screening of anticancer drugs, *Molecular Pharmaceutics*, 2020, **17**, 4709-4714, 10.1021/acs.molpharmaceut.0c00791

Sprick RS, Chen Z, Cowan AJ, Bai Y, Aitchison CM, Fang Y, **Zwijnenburg MA**, Cooper AI, Wang X, Water oxidation with cobalt-loaded linear conjugated polymer photocatalysts, *Angewandte Chemie International Edition*, 2020, **59**, 18695-18700, 10.1002/ange.202008000

Steenro R, Minoia A, Gimenez-Lopez MC, **Blunt MO**, Champness NR, Lazzaroni R, Mali KS, De Feyter S, Molecular dopant determines the structure of a physisorbed self-assembled molecular network, *Chemical Communications*, 2021, **57**, 1454-1457, 10.1039/d0cc07338e

Stojanovski G, Dobrijevic D, **Hailes HC**, Ward JM, Identification and catalytic properties of new epoxide hydrolases from the genomic data of soil bacteria, *Enzyme and Microbial Technology*, 2020, **139**, 109592, 10.1016/j.enzmictec.2020.109592

Subrizi F, Wang Y, Thair B, Méndez-Sánchez D, Roddan R, Cárdenas-Fernández M, Siegrist J, Richter M, Andexer JN, Ward JM, **Hailes HC**, Multienzyme one-pot cascades incorporating methyltransferases for the strategic diversification of tetrahydroisoquinoline alkaloids, *Angewandte Chemie International Edition*, 2021, **60**, 18673-18679, 10.1002/ange.202104476

Suleimenova D, Arabnejad H, Edeling WN, Coster D, Luk OO, Lakhilili J, Jancauskas V, Kulczewski M, Veen L, Ye D, Zun P, Krzhizhanovskaya V, Hoekstra A, Crommelin D, **Coveney PV**, Groen D, Tutorial applications for Verification, Validation and Uncertainty Quantification using VECMA toolkit, *Journal of Computational Science*, 2021, **53**, 101402, 10.1016/j.jocs.2021.101402

Suter TM, Carrero NR, Rana Z, **Clancy AJ**, Heitzmann M, Guetaz L, Shearing PR, Howard CA, Gebel G, **McMillan PF**, Shaffer MSP, Brett DJL, Spacers to improve performance and porosity of graphene based polymer electrolyte fuel cells, *ECS Transactions*, 2020, **98**, 141-146, 10.1149/09802.0141ecst

Swallow JEN, **Palgrave RG**, Murgatroyd PAE, **Regoutz A**, Lorenz M, Hassa A, Grundmann M, von Wenckstern H, Varley JB, Veal TD, Indium Gallium Oxide alloys: electronic structure, optical gap, surface space charge, and chemical trends within common-cation semiconductors, *ACS Applied Materials & Interfaces*, 2021, **13**, 2807-2819, 10.1021/acsami.0c16021

Swallow JEN, Vorwerk C, Mazzolini P, Vogt P, Bierwagen O, Karg A, Eickhoff M, Schörmann J, Wagner MR, Roberts JW, Chalker PR, Smiles MJ, Murgatroyd P, Razek SA, Lebens-Higgins ZW, Piper LFJ, Jones LAH, Thakur PK, Lee T-L, Varley JB, Furthmüller J, Draxl C, Veal TD, **Regoutz A**, Influence of polymorphism on the electronic structure of Ga2O3, *Chemistry of Materials*, 2020, **32**, 8460-8470, 10.1021/acs.chemmater.0c02465

Syed AJ, **Anderson JC**, Applications of bioluminescence in biotechnology and beyond, *Chemical Society Reviews*, 2021, **50**, 5668-5705, 10.1039/d0cs01492c

Szijj P, **Chudasama V**, The renaissance of chemically generated bispecific antibodies, *Nature Reviews Chemistry*, 2021, **5**, 78-92, 10.1038/s41570-020-00241-6

Szijj PA, Kostadinova KA, Spears RJ, **Chudasama V**, Tyrosine bioconjugation - an emergent alternative, *Organic & Biomolecular Chemistry*, 2020, **18**, 9018-9028, 10.1039/d0ob01912g

Szalai AM, Siarry B, Lukin J, Williamson DJ, Unsain N, Cáceres A, Pilo-Pais M, Acuna G, Refojo D, Owen DM, **Simoncelli S**, Stefani FD, Three-dimensional total-internal reflection fluorescence nanoscopy with nanometric axial resolution by photometric localization of single molecules, *Nature Communications*, 2021, **12**, 517, 10.1038/s41467-020-20863-0

Szpara R, Alexander G, **Porter M**, **Hailes H**, **Sheppard T**, Regioselective Dehydration of Sugar Thioacetals under Mild Conditions, *Organic Letters*, 2021, **23**, 2488-2492, 10.1021/acs.orglett.1c00424

Taj S, Rosu-Finsen A, McCoustra MRS, Impact of surface heterogeneity on IR line profiles of adsorbed carbon monoxide on models of interstellar grain surfaces, *Monthly Notices of the Royal Astronomical Society*, 2021, **504**, 5806-5812, 10.1093/mnras/stab1174



Tan JZY, Gavrielides S, Belekoukia M, Thompson WA, Negahdar L, xia F, Maroto-Valer M, **Beale AM**, Synthesis of  $\text{TiO}_{2-x}/\text{W}_{18}\text{O}_{49}$  Hollow Double-shell and Core-shell Microspheres for  $\text{CO}_2$  Photoreduction under Visible Light, *Chemical Communications*, 2020, **56**, 12150-12153, 10.1039/d0cc04036c

Tanner AJ, Wen B, Ontaneda J, Zhang Y, Grau-Crespo R, **Fielding HH**, Selloni A, **Thornton G**, Polaron-adsorbate coupling at the  $\text{TiO}_2(110)$ -carboxylate interface, *The Journal of Physical Chemistry Letters*, 2021, **12**, 3571-3576, 10.1021/acs.jpcllett.1c00678

Tanner AJ, Wen B, Zhang Y, Liu L-M, **Fielding HH**, Selloni A, **Thornton G**, Photoexcitation of bulk polarons in rutile  $\text{TiO}_2$ , *Physical Review B*, 2021, **103**, L121402, 10.1103/physrevb.103.L121402

Tappan BA, Zhu B, Cottingham P, Mecklenburg M, **Scanlon DO**, Brutchey RL, Crystal structure of colloiddally prepared metastable  $\text{Ag}_2\text{Se}$  nanocrystals, *Nano Letters*, 2021, **21**, 5881-5887, 10.1021/acs.nanolett.1c02045

Tian X, De Pace C, Ruiz-Perez L, Chen B, Su R, Zhang M, Zhang R, Zhang Q, Wang Q, Zhou H, Wu J, Zhang Z, Tian Y, **Battaglia G**, A cyclometalated Iridium (III) complex as a microtubule probe for correlative super-resolution fluorescence and electron microscopy, *Advanced Materials*, 2020, **32**, 2003901, 10.1002/adma.202003901

Tian X, Leite DM, Scarpa E, Nyberg S, Fullstone G, Forth J, Matias D, Apriceno A, Poma A, Duro-Castano A, Vuyyuru M, Harker-Kirschneck L, Šarić A, Zhang Z, Xiang P, Fang B, Tian Y, Luo L, Rizzello L, **Battaglia G**, On the shuttling across the blood-brain barrier via tubule formation: Mechanism and cargo avidity bias, *Science Advances*, 2020, **6**, eabc4397, 10.1126/sciadv.abc4397

Tinker HR, Bhide MA, Magliocca E, Miller TS, **Knapp CE**, Synthetic tethered silver nanoparticles on reduced graphene oxide for alkaline oxygen reduction catalysis, *Journal of Materials Science*, 2021, **56**, 6966-6976, 10.1007/s10853-020-05711-2

To KC, Ben-Jaber S, **Parkin IP**, Recent developments in the field of explosive trace detection, *ACS nano*, 2020, **14**, 10804-10833, 10.1021/acsnano.0c01579

Tran T, **Worth GA**, Robb MA, Control of nuclear dynamics in the benzene cation by electronic wavepacket composition, *Communications Chemistry*, 2021, **4**, 48, 10.1038/s42004-021-00485-3

Vamvakeros A, Coelho AA, Matras D, Dong H, Odarchenko Y, Price SWT, Butler KT, Gutowski O, Dippel A-C, Zimmermann M, Martens I, Drnec J, **Beale AM**, Jacques SDM, DLSR: a solution to the parallax artefact in X-ray diffraction computed tomography data, *Journal of Applied Crystallography*, 2020, **53**, 1531-1541, 10.1107/s1600576720013576

Vassaux M, Gopalakrishnan K, Sinclair RC, Richardson RA, **Coveney PV**, Accelerating heterogeneous multiscale simulations of advanced materials properties with graph-based clustering, *Advanced Theory and Simulations*, 2020, **4**, 2000234, 10.1002/adts.202000234

Vassaux M, Wan S, Edeling W, **Coveney PV**, Ensembles are required to handle aleatoric and parametric uncertainty in molecular dynamics simulation, *Journal of Chemical Theory and Computation*, 2021, **17**, 5187-5197, 10.1021/acs.jctc.1c00526

Veal TD, **Scanlon DO**, Kostecki R, Arca E, Accelerating the development of new solar absorbers by photoemission characterization coupled with density functional theory, *Journal of Physics: Energy*, 2021, **3**, 032001, 10.1088/2515-7655/abebc9

Venezia B, Cao E, Matam SK, Waldron C, Cibir G, Gibson EK, Golunski S, Wells PP, Silverwood I, **Catlow CRA**, **Sankar G**, Gavriilidis A, Silicon microfabricated reactor for operando XAS/DRIFTS studies of heterogeneous catalytic reactions, *Catalysis Science & Technology*, 2020, **10**, 7842-7856, 10.1039/d0cy01608j

Venezia B, Panariello L, Biri D, Shin J, Damilos S, Radhakrishnan ANP, **Blackman C**, Gavriilidis A, Catalytic Teflon AF-2400 membrane reactor with adsorbed *ex situ* synthesized Pd-based nanoparticles for nitrobenzene hydrogenation, *Catalysis Today*, 2021, **362**, 104-112, 10.1016/j.cattod.2020.03.062

Vicente-Rodríguez M, Singh N, Turkheimer F, Peris-Yague A, Randall K, Veronese M, Simmons C, Karim Haji-Dheere A, Bordoloi J, **Sander K**, Awais RO, Årstad E, Consortium N, Cash D, Parker CA, Resolving the cellular specificity of TSPO imaging in a rat model of peripherally-induced neuroinflammation, *Brain, Behavior, and Immunity*, 2021, 10.1016/j.bbi.2021.05.025

Acree Jr. WE, Churchill B, **Abraham MH**, Comments on “Classification of biphasic solvent systems according to Abraham descriptors for countercurrent chromatography”, *Journal of Chromatography A*, 2020, **1618**, 460889, 10.1016/j.chroma.2020.460889

Wall A, Wills AG, Forte N, Bahou C, Bonin L, Nicholls K, Ma MT, **Chudasama V**, **Baker JR**, One-pot thiol–amine bioconjugation to maleimides: simultaneous stabilisation and dual functionalisation, *Chemical Science*, 2020, **11**, 11455-11460, 10.1039/d0sc05128d

Wan S, Bhati AP, Zasada SJ, **Coveney PV**, Rapid, accurate, precise and reproducible ligand–protein binding free energy prediction, *Interface Focus*, 2020, **10**, 20200007, 10.1098/rsfs.2020.0007

Wan S, Kumar D, Ilyin V, Al Homsy U, Sher G, Knuth A, **Coveney PV**, The effect of protein mutations on drug binding suggests ensuing personalised drug selection, *Scientific Reports*, 2021, **11**, 13452, 10.1038/s41598-021-92785-w

Wan S, Potterton A, Hussein FS, Wright DW, Heifetz A, Malawski M, Townsend-Nicholson A, **Coveney PV**, Hit-to-lead and lead optimization binding free energy calculations for G protein-coupled receptors: Free energy calculations for GPCRs, *Interface Focus*, 2020, **10**, 20190128, 10.1098/rsfs.2019.0128

Wan S, Sinclair RC, **Coveney PV**, Uncertainty quantification in classical molecular dynamics, *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 2021, **379**, 20200082, 10.1098/rsta.2020.0082

Wang M, Sanchez-Perez C, Habib F, **Blunt MO**, **Carmalt CJ**, Scalable production of ambient stable hybrid bismuth-based materials: AACVD of phenethylammonium bismuth iodide films, *Chemistry – A European Journal*, 2021, **27**, 9406-9413, 10.1002/chem.202100774

Wang S, He M, Walter M, Kravchyk KV, Kovalenko MV, Monodisperse  $\text{CoSb}$  nanocrystals as high-performance anode material for Li-ion batteries, *Chemical Communications*, 2020, **56**, 13872-13875, 10.1039/d0cc06222g

Wang X, Lu Y, Zhang Q, Wang K, **Carmalt CJ**, **Parkin IP**, Zhang Z, Zhang X, Durable fire retardant, superhydrophobic, abrasive resistant and air/UV stable coatings, *Journal of Colloid and Interface Science*, 2021, **582**, 301-311, 10.1016/j.jcis.2020.07.084

Ward S, Isaacs MA, Gupta G, Mamlouk M, Pramana SS, Boosting the oxygen evolution activity in non-stoichiometric praseodymium ferrite-based perovskites by A site substitution for alkaline electrolyser anodes, *Sustainable Energy & Fuels*, 2020, **5**, 154-165, 10.1039/d0se01278e

Warne EM, Downes-Ward B, Woodhouse J, **Parkes MA**, Springate E, Pearcy PAJ, Zhang Y, Karras G, Wyatt AS, Chapman RT, Minns RS, Photodissociation dynamics of methyl iodide probed using femtosecond extreme ultraviolet photoelectron spectroscopy, *Physical Chemistry Chemical Physics*, 2020, **22**, 25695-25703, 10.1039/d0cp03478a

Weaving JS, Lim A, Millichamp J, Neville TP, Ledwoch D, Kendrick E, **McMillan PF**, Shearing PR, Howard CA, Brett DJL, Elucidating the sodiation mechanism in hard carbon by operando raman spectroscopy, *ACS Applied Energy Materials*, 2020, **3**, 7474-7484, 10.1021/acsaem.0c00867

Westbrook RJE, Xu W, Liang X, Webb T, **Clarke TM**, Haque SA, 2D Phase purity determines charge-transfer yield at 3D/2D lead halide perovskite heterojunctions, *The Journal of Physical Chemistry Letters*, 2021, **12**, 3312-3320, 10.1021/acs.jpcllett.1c00362

Williams GT, **Haynes CJE**, Fares M, Caltagirone C, Hiscock JR, Gale PA, Advances in applied supramolecular technologies, *Chemical Society Reviews*, 2021, **50**, 2737-2763, 10.1039/d0cs00948b

Williams I, Lee S, Apriceno A, Sear RP, **Battaglia G**, Diffusioosmotic and convective flows induced by a nonelectrolyte concentration gradient, *Proceedings of the National Academy of Sciences of the United States of America*, 2021, **118**, e2025408118, 10.1073/pnas.2025408118

Wilson RL, Macdonald TJ, Lin CT, Xu S, Taylor A, **Knapp CE**, Guldin S, McLachlan MA, **Carmalt CJ**, **Blackman CS**, Chemical vapour deposition (CVD) of nickel oxide using the novel nickel dialkylaminoalkoxide precursor  $[\text{Ni}(\text{dmamp}')_2]$  ( $\text{dmamp}' = 2\text{-dimethylamino-2-methyl-1-propanolate}$ ), *RSC Advances*, 2021, **11**, 22199-22205, 10.1039/d1ra03263a

**Woodley SM**, Day GM, **Catlow R**, Structure prediction of crystals, surfaces and nanoparticles, *Philosophical transactions. Series A, Mathematical, physical, and engineering sciences*, 2020, **378**, 20190600, 10.1098/rsta.2019.0600

Wu Y, Zhang Q, **Xu Y**, Xu R, Li L, Li Y, Zhang C, Zhao H, Wang S, Kaiser U, Lei Y, Enhanced potassium storage capability of two-dimensional transition-metal chalcogenides enabled by a collective strategy, *ACS Applied Materials and Interfaces*, 2021, **13**, 18838-18848, 10.1021/acsaami.1c01891

Xu S, Han X, Ma Y, Duong TD, Lin L, Gibson EK, Sheveleva A, Chansai S, Walton A, Ngo DT, Frogley MD, Tang CC, Tuna F, McInnes EJJ, **Catlow CRA**, Hardacre C, Yang S, Schröder M, Catalytic decomposition of  $\text{NO}_2$  over a copper-decorated metal–organic framework by non-thermal plasma, *Cell Reports Physical Science*, 2021, **2**, 100349, 10.1016/j.xcrp.2021.100349

**Xu Y**, Bahmani F, Wei R, Pyrrhotite  $\text{Fe}_{1-x}\text{S}$  microcubes as a new anode material in potassium-ion batteries, *Microsystems and Nanoengineering*, 2020, **6**, 75, 10.1038/s41378-020-00188-0

**Xu Y**, Sumboja A, Groves A, Ashton T, Zong Y, **Darr JA**, Enhancing bifunctional catalytic activity of cobalt-nickel sulfide spinel nanocatalysts through transition metal doping and its application in secondary zinc-air batteries, *RSC Advances*, 2020, **10**, 41871-41882, 10.1039/d0ra08363a

Xu Z, **Palgrave RG**, Hayward MA,  $\text{LaSrCo}_{0.5}\text{Rh}_{0.5}\text{O}_{3.25}$  and  $\text{LaSrNi}_{0.5}\text{Rh}_{0.5}\text{O}_{3.25}$ : Topochemically reduced, mixed valence Rh(I)/Rh(III) oxides, *Inorganic Chemistry*, 2020, **59**, 13767-13773, 10.1021/acs.inorgchem.0c02131

Yamamoto T, Oswald IWH, Savory CN, Ohmi T, Koegel AA, **Scanlon DO**, Kageyama H, Neilson JR, Structure and optical properties of layered perovskite  $(\text{MA})_2\text{Pb}_{1-x}\text{Br}_x(\text{SCN})_2$  ( $0 \leq x < 1.6$ ), *Inorganic Chemistry*, 2020, **59**, 17379-17384, 10.1021/acs.inorgchem.0c02686

Yang H, Savory CN, Morgan BJ, **Scanlon DO**, Skelton JM, Walsh A, Chemical trends in the lattice thermal conductivity of  $\text{Li}(\text{Ni}, \text{Mn}, \text{Co})\text{O}_2$  (NMC) Battery Cathodes, *Chemistry of Materials*, 2020, **32**, 7542-7550, 10.1021/acs.chemmater.0c02908

Yap SY, Frias B, Wren MC, Schöll M, Fox NC, Årstad E, Lashley T, **Sander K**, Discriminatory ability of next-generation tau PET tracers for Alzheimer’s disease, *Brain*, 2021, 10.1093/brain/awab120

Yilmaz M, Handoko AD, **Parkin IP**, **Sankar G**, Probing the electronic and geometric structures of photoactive electrodeposited  $\text{Cu}_2\text{O}$  films by X-ray absorption spectroscopy, *Journal of Catalysis*, 2020, **389**, 483-491, 10.1016/j.jcat.2020.06.021

Yu T, Li Z, Jones W, Liu Y, He Q, Song W, Du P, Yang B, An H, Farmer DM, Qiu C, Wang A, Weckhuysen BM, **Beale AM**, Luo W, Identifying key mononuclear Fe species for low-temperature methane oxidation, *Chemical Science*, 2021, **12**, 3152-3160, 10.1039/d0sc06067d

Yue D, Acree Jr. WE, **Abraham MH**, Applications of Abraham solvation parameter model: estimation of the lethal median molar concentration of the antiepileptic drug levetiracetam towards aquatic organisms from measured solubility data, *Physics and Chemistry of Liquids*, 2019, **58**, 302-308, 10.1080/00319104.2019.1584801

Zasada SJ, Wright DW, **Coveney PV**, Large-scale binding affinity calculations on commodity compute clouds, *Interface Focus*, 2020, **10**, 20190133, 10.1098/rsfs.2019.0133

Zaw Thin M, Allan H, Bofinger R, Kostelec TD, Guillaume S, Connell JJ, Patrick PS, **Hailes HC**, **Tabor AB**, Lythgoe MF, Stuckey DJ, Kalber TL, Multi-modal imaging probe for assessing the efficiency of stem cell delivery to orthotopic breast tumours, *Nanoscale*, 2020, **12**, 16570-16585, 10.1039/d0nr03237a

Zhang C, **Xu Y**, He K, Dong Y, Zhao H, Medenbach L, Wu Y, Balducci A, Hannappel T, Lei Y, Polyimide@Ketjenblack composite: a porous organic cathode for fast rechargeable potassium-ion batteries, *Small*, 2020, **16**, 2002953, 10.1002/smll.202002953

Zhang S, Li ML, Jiang M, Xiao HY, **Scanlon DO**, Zu XT, Formation and migration of vacancy defects in GeSe and SnSe, *Journal of Physics B: Atomic, Molecular and Optical Physics*, 2021, **54**, 35003, 10.1088/1361-6455/abd9fd

Zhang Y, Kirs A, Ambroz F, Lin CT, Bati ASR, **Parkin IP**, Shapter JG, Batmunkh M, Macdonald TJ, Ambient fabrication of organic–inorganic hybrid perovskite solar cells, *Small Methods*, 2020, **5**, 2000744, 10.1002/smt.202000744

Zhang Y, Li B, Wang Z, Tian S, Liu B, Zhao X, Li N, **Sankar G**, Wang S, Facile Preparation of  $\text{Zn}_2\text{V}_2\text{O}_7\text{--VO}_2$  composite films with enhanced thermochromic properties for smart windows, *ACS Applied Electronic Materials*, 2021, **3**, 2224-2232, 10.1021/acsaelm.1c00176

Zhao D, Li J, Sathasivam S, **Carmalt CJ**, n-Type conducting P doped ZnO thin films via chemical vapor deposition, *RSC Advances*, 2020, **10**, 34527-34533, 10.1039/d0ra05667g

Zhao J, Méndez-Sánchez D, Roddan R, Ward JM, **Hailes HC**, Norcoclaurine synthase-mediated stereoselective synthesis of 1,1’-disubstituted, spiro- and bis-tetrahydroisoquinoline alkaloids, *ACS Catalysis*, 2021, **11**, 131-138, 10.1021/acscatal.0c04704

Zhao S, Yang M, Tan Y, Brett DJL, He G, **Parkin IP**, Facile room-temperature synthesis of cobalt sulphide for efficient oxygen evolution reaction, *Multifunctional Materials*, 2021, **4**, 025001, 10.1088/2399-7532/abfeb8

Zhao T, Gibson QD, Daniels LM, **Slater B**, **Cora F**, Prediction of higher thermoelectric performance in  $\text{BiCuSeO}$  by weakening electron-polar optical phonon scattering, *Journal of Materials Chemistry A*, 2020, **8**, 25245-25254, 10.1039/d0ta08839k

Zhuk S, Wong TKS, Petrovic M, Kymakis E, Hadke SS, Lie S, Wong LH, Sonar P, Dey A, Krishnamurthy S, Dalapati GK, Solution-Processed Pure Sulfide  $\text{Cu-2(ZnO.6CdO4)}$   $\text{SnS}_4$  Solar Cells with Efficiency 10.8% Using Ultrathin  $\text{CuO}$  Intermediate Layer, *Solar RRL*, 2020, **4**, 2000293, 10.1002/solr.202000293



# Grants

**Investigator:** Prof Robert Palgrave  
**Title:** Long HBar 2 - Lead-free halometallates – the next generation hybrid photovoltaic absorber materials  
**Sponsor:** Innovate UK  
**Value:** £249,703.00  
**Period:** 01/10/2020 to 30/09/2023

**Investigator:** Dr Rebecca Ingle  
**Title:** Capturing Dynamics at the Heart of Catalysis with Ultrafast X-ray Spectroscopy  
**Sponsor:** Royal Society  
**Value:** £19,214.30  
**Period:** 01/09/2020 to 31/01/2022

**Investigator:** Prof Ivan Parkin  
**Title:** Managing Covid-19 Complications in ICU: Antimicrobial Endotracheal Tubes for Ventilated Patients  
**Sponsor:** EPSRC IAA  
**Value:** £93,423.00  
**Period:** 13/01/2021 to 01/02/2022

**Investigator:** Prof Helen Hailes  
**Title:** Selective Methylation And Alkylation Using Methyl Transferases  
**Sponsor:** Almac Sciences Limited  
**Value:** £13,600.00  
**Period:** 28/09/2020 to 30/09/2024

**Investigator:** Prof Graham Worth  
**Title:** Photoexcited DNA Nucleobases: Towards Complete Quantum Dynamics Simulations Including Solvent  
**Sponsor:** The Royal Society  
**Value:** £12,000.00  
**Period:** 11/01/2021 to 10/01/2023

**Investigator:** Dr Caroline Knapp  
**Title:** Designer Aluminium Precursors For The Inkjet Printing Of Electrical Circuits  
**Sponsor:** EPSRC  
**Value:** £415,688  
**Period:** 01/04/2021 - 31/03/2024

**Investigator:** Prof Jawwad Darr  
**Title:** Discovery And Scale Up Of New Industrial Nanomaterials  
**Sponsor:** QinetiQ Group PLC  
**Value:** £28,600  
**Period:** 01/10/2019 - 30/9/2023

**Investigator:** Prof Christopher Blackman  
**Title:** Atomic Layer Deposition Of Single Platinum Atom Catalysts On Nanostructured Cupreous Oxide Supports For Photoelectrochemical Water Splitting  
**Sponsor:** Daphne Jackson Memorial Fellowships Trust  
**Value:** £57,763.5  
**Period:** 07/06/2021 - 06/06/2023

**Investigator:** Prof Ivan Parkin  
**Title:** Synthesis of biodegradable polymers in collaboration with Nanoforce Technology Ltd  
**Sponsor:** EPSRC  
**Value:** £5,000  
**Period:** 03/05/2021 - 30/06/2021

**Investigator:** Prof Andrew Beale  
**Title:** Selective CO2 conversion to renewable methanol through innovative heterogeneous catalyst systems optimized for advanced hydrogenation technologies (microwave, plasma and magnetic induction)  
**Sponsor:** European Commission  
**Value:** £479,246.00 (€599,057.50)  
**Period:** 01/05/2021 - 30/04/2025

**Investigator:** Prof Peter Coveney  
**Title:** Software Environment For Actionable & VVUQ-evaluated Exascale Applications  
**Sponsor:** EPSRC (Strategic Priorities Fund)  
**Value:** £484,365  
**Period:** 02/08/2021 to 01/08/2024

**Investigator:** Prof Jawwad Darr  
**Title:** Scale-up Production and Pre-commercial Evaluation of High Value Rare Earth Xray and Neutron Scintillator Powders with AWE  
**Sponsor:** EPSRC Impact Acceleration Account (IAA)  
**Value:** £50,000.00  
**Period:** 01/10/2021 - 31/03/2022

**Investigator:** Prof Alethea Tabor  
**Title:** Interrogating the nisin: lipid II interaction: a chemical biology approach  
**Sponsor:** EPSRC  
**Value:** £759,212.97  
**Period:** 01/03/2021 - 29/02/2024

**Investigator:** Prof Alethea Tabor  
**Title:** Targeted theragnostic liposomal probes for imaging and treatment of Acute Myeloid Leukaemia (AML)  
**Sponsor:** CRUK - City of London 2021 Development Fund Award  
**Value:** £24,000.00  
**Period:** 01/04/2021 - 31/03/2022

**Investigator:** Dr Yang Xu  
**Title:** Understanding amorphization in materials for calcium-ion storage  
**Sponsor:** Leverhulme Trust  
**Value:** £201,425  
**Period:** 01/10/2021 - 30/09/2024

**Investigator:** Prof David Scanlon  
**Title:** Michael Computer Running Costs  
**Sponsor:** Faraday Institute  
**Value:** £410,995  
**Period:** 01/03/2021 - 28/02/2024

**Investigator:** Prof Helen Fielding  
**Title:** Femtosecond time-resolved spectroscopy of bioluminescence emitters  
**Sponsor:** Coherent Europe BV  
**Value:** £37,500.00  
**Period:** 01/10/2021 - 30/09/2024

**Investigator:** Prof Vijay Chudasama  
**Title:** Bioconjugation: Novel Reagents and Strategies for Cysteine and Disulfide Modification  
**Sponsor:** MSD  
**Value:** £35,050  
**Period:** 01/10/2021 - 30/09/2025

**Investigator:** Dr Dejan-Kresimir Bucar  
**Title:** Crystalline and stable covalent organic frameworks based on carbon-carbon bonds  
**Sponsor:** Leverhulme Trust  
**Value:** £259,276  
**Period:** 01/09/2021 - 31/08/2024

**Investigator:** Dr Fabrizia Foglia  
**Title:** Advanced neutron scattering techniques to understand and improve performance in membrane nanotechnology  
**Sponsor:** EPSRC  
**Value:** £1,233,592.20  
**Period:** 01/09/2021 - 31/08/2026

**Investigator:** Prof Katherine Holt  
**Title:** Diamond and Metal Photo-Electrocatalysts for Hydrogen Evolution and Carbon Dioxide Reduction  
**Sponsor:** European Commission  
**Value:** £179,947.01 (€224,933.76)  
**Period:** 01/01/21 - 31/12/22

**Investigator:** Prof Stephen Price  
**Title:** Heterogeneous Radial Reactions of Relevance to the Interstellar Medium  
**Sponsor:** Royal Society of Chemistry  
**Value:** £9,959  
**Period:** 01/10/2021 to 30/11/2021

**Investigator:** Prof Peter Coveney  
**Title:** FM-WP1 Numerical Representation: Study Of Uncertainty Quantification Techniques (Project NEPTUNE)  
**Sponsor:** UKAEA UK Atomic Energy Authority  
**Value:** £53,279  
**Period:** 04/01/2021 - 31/07/2021

**Investigator:** Prof Helen Fielding  
**Title:** Ultrafast Photochemical Dynamics in complex environments  
**Sponsor:** EPSRC  
**Value:** £1,709,105.06  
**Period:** 01/06/2021 to 31/05/2027

**Investigator:** Dr Giorgio Volpe  
**Title:** Contactless Droplet Manipulation for Highly Aligned Organic Semiconductors  
**Sponsor:** EPSRC  
**Value:** £941,347.68  
**Period:** 01/01/2022 to 31/12/2024

**Investigator:** Prof Ivan Parkin  
**Title:** A durable and scalable anti-soiling coating for solar modules  
**Sponsor:** EPSRC  
**Value:** £453,318.01  
**Period:** 01/10/2021 to 30/09/2024

**Investigator:** Prof Helen Hailes  
**Title:** Compostable Plastics: Unlocking Existing Barriers To Systems Change  
**Sponsor:** NERC  
**Value:** £235,091.11  
**Period:** 01/11/2020 to 31/10/2023

# Staff

## Departmental Structure

**Head of Department**  
C.J. Carmalt

**Deputy Head of Department (Teaching)**  
D.W. Lewis

**Deputy Head of Department (Operations)**  
S.D. Price

**Head of Physical Chemistry & Virtual Computational Chemistry Section**  
G.A. Worth

**Head of Materials & Inorganic Chemistry Section**  
F. Cora

**Head of Organic Chemistry & Chemical Biology Section**  
A.B. Tabor

## Computational Chemistry

**Professors:**  
C.R.A. Catlow  
P.V. Coveney  
S.L. Price  
B. Slater  
D. Scanlon  
S. Woodley  
G. Worth  
M. Zwijnenburg

**Readers and Senior Lecturers**  
R.G. Bell  
D.W. Lewis

**Royal Society URF and Lecturer**  
T. Hele

**Principal Research Associate**  
A. Sokol

**Ramsay Fellow**  
C. Savory

**Marie Curie Fellow**  
D. Dey

**Research Associates**  
A. Bhati  
Y.S. Choi  
M. Einhorn  
S. Gomez Rodriguez  
K. Gopalakrishnan  
J. Guan  
Q. Liao  
B. Mant  
H. Martin  
J. McCullough  
A. Prentice  
A. Van Haeften  
A. Wade  
S. Wan  
B. Zhu

## Materials & Inorganic Chemistry

**Professors**  
A. Beale  
C. Blackman  
C.J. Carmalt  
F. Cora  
J.A. Darr  
P.F. McMillan  
I. P. Parkin  
R. Palgrave  
G. Sankar  
A. Sella

**Readers and Senior Lecturers**  
J. Cockcroft

**Associate Professor**  
G.L. Davies

**Lecturers**  
C. E. Knapp  
Y. Xu  
A. Regoutz

**Ramsay Fellow**  
A. Clancy  
G. Hwang

**EPSRC Fellow**  
F. Foglia

**Marie Curie Fellow**  
L. Negahdar

**Daphne Jackson Fellow**  
S. Ashraf

**Horsell Fellow**  
S. Sathasivam

**Research Associates**  
T. Ashton  
H. Bhatia  
F. Chang  
A. Dey  
R. Gaifulina  
M. Isaacs  
I. Lezcano Gonzalez  
A. Piriya

**Senior Research Associate**  
K. Page  
R. Quesada Cabrera  
M. Vickers

## Organic & Chemical Biology

**Professors**  
J.C. Anderson  
E. Arstad  
J.R. Baker  
S. Caddick  
V. Chudasama  
H.C. Hailes  
S. Howorka  
C.M. Marson  
M. Porter  
M. Powner  
T. Sheppard  
A.B. Tabor

**Associate Professor**  
D. Macmillan  
B. Schroeder

**Lecturers**  
K. Bucar  
K. Sander  
C. Haynes

**Royal Society URF**  
J. Attwater



#### Marie Curie Fellow

A. Alves Magalhaes  
L. Rochet  
F. Thoreau

#### NMR Manager and Principal Research Fellow

A. Aliev

#### Senior Research Associates

H. Allan  
H. Britton

#### Research Associates

C. Bahou  
N. Barnes  
M. Bawn  
J. Burns  
C. Chang  
L. Cowen  
A. Dorey  
P. Finn  
S. Hassell-Hart  
K. Hawkins  
S. Islam  
L. Leipold  
F. Ma  
R. Procter  
J. Singh  
R. Spears  
S. St John-Campbell  
F. Subrizi  
B. Szulc  
D. Whitaker  
Y. Xing  
K. Yang  
S. Yap

## Physical Chemistry

#### Professors

G. Battaglia  
D.J. Caruana  
H.H. Fielding  
F.L. Gervasio  
K.B. Holt  
S.D. Price  
C.G. Salzmann  
G. Thornton  
A.S. Wills

#### Associate Professors

T. Clarke  
G. Volpe

#### Senior Lecturers

D.M. Rowley

#### Lecturers

M. Blunt  
R. Ingle

#### Royal Society Dorothy Hodgkin Fellow & Lecturer

S. Simoncelli

#### Ramsay Fellow

J. Forth

#### Marie Curie Fellow

S. Heijnen  
S. Kumar Padamati

#### Senior Research Associate

M. Parkes

#### Research Associates

S. Acosta Gutierrez  
D. Cecchin  
J. Davies  
Y. Deng  
L. Ellis-Gibblings  
A. Kuzmanic  
D Moreira Leite  
A. Rosu-Finsen  
E. Scarpa  
M. Scholz

## Teaching

#### Director of Teaching and Learning

J. Baker

#### Director of Postgraduate Studies

J.C. Anderson

#### Director of Undergraduate Studies

D.W. Lewis

#### EngD Coordinator

Z. Du

#### Postgraduate Taught Tutor

D.J. Caruana

#### Undergraduate Admissions Tutor

M. Blunt

#### Associate professor (Teaching)

S.E. Potts

#### Lecturer (Teaching)

T. Alhilfi  
V. Hilborne  
A. Roffey

#### Associate Lecturers (Teaching)

J.L. Kiappes Jr.  
L. Munday  
R. Riley  
M. Rivera

#### PhD Students

Jamal Abdul Nasir, Samuel Ackerley, Nehaal Ahmed, Maryam Alghamdi, Michael Allan, Lisa Allen, Safa Almadhi, Alvaro Alves Magalhaes, Esther Ambrose-Dempster, Filip Ambroz, Divya Amin, Sam Armenta Butt, Zuharia Arshad, Solomon Asghar, Jude Ayogu, Calise Bahou, Lolade Bamgbelu, Abid Barat, Valentino Barbieri, Szymon Bartus, Jessica Batey, Archana Bhartiya, Malavika Bhide, Phyllida Britton, Katarina Brlec, Joseph Broughton, Joseph Buckley, Ayrton Burgess, Emma Campbell, Eve Carter, Sam Cassidy, Alvaro Castillo Bonillo, Jiayi Cen, John Chapman-Fortune, Jintao Chen, Junyang Chen, Sining Chen, Bharvi Chikani, Yasmin Choaie, Georgia Christopoulou, Alina Chrzastek, Ivan Clayson, Arran Collis, Benjamin Colville, Peixi Cong, Jaymee Coonjobeeharry, Matt Cross, Andrew Cummings, Chiara Cursi, Billy Darling, Gemma Davison, Cesare De Pace, Alec Desmoutier, Simran Kaur Dhaliwal, Xindi Diao, Yiming Ding, Haobo Dong, Teng Dong, Sam Douglas, Zacharie Edwards, Rhys Evans, Tim Evans, Jasper Fairchild, Daniela Farmer, Danial Farooq, Jiangqi Feng, Nathalie Fernando, Panagiotis Fikas, Georgia Fleet, Mandy Fong, William Fortune, Alexander Furby, Yiannis Galdadas, Lavan Ganeshkumar, Erze Gao, Alessia Gentili, Elena Georgiou, Madeleine Georgopoulou, Alexander Gheorghiu, William Goldring, Hristo Gonev, Alexandra Groves, Junwen Gu, Bowen Guan, Jian Guo, Junjun Guo, Xiaoxia Guo, Faiza Habib, Siriney Halukeerthi, James Hammerton, Muhammed Haque, Mark Hardmeier Samame, Isabelle Heath-Apostolopoulos, Christopher Heaton, Alice Henley, Luisa Herring-Rodriguez, Daniel Hewitt, Katie Hobson, Qing Hou, Xueying Hu, Jingle Huang, Martin Hutereau, James Hutton, Barbara Ibarzo Yus, Mohamed Ibrahim, Jameel Imran, Ana-Maria Ivanus, Clement Jacquot, Beatriz Janeiro Ferraz, Faiza Javaid, Woongkyu Jee, Yiding Jiao, Tabitha Jones, Curran Kalha, Julie Kalmoni, Tonggih Kang, Maham Karim, Sean Kavanagh, Robin Kerr, Ahmad Khan, Zahra Khan, Zaibunisa Khan, Aaron King, Hiral Kotak, Stefan Kucharski, Gogulan Kugan, Charles Lamb, Hugues Lambert, Roxanna Lee, Viliyana Lewis, Diyuan Li, Jianwei Li, Juntao Li, Yixuan Li, Jiaqi Lin, Quanyao Lin, Runjia Lin, Karolina Lisowska, Jia Liu, Longxiang Liu, Yuhan Liu, Sharp Lo, Isa Tristan Lough, Yi Lu, Dominykas Lukauskis, Richard Lunn,

Minyan Lyu, Sinead Maher, Roshni Malde Gabriele Marchello, Liam Martin, Fathima Marzook, Henry McGhee, Natalie McLeod, Kristian Mears, Saf Mendez, Tina Miao, Katherine Milton, Manesh Mistry, Shreya Mrig, Werner Muller Roa, Aamina Murtza, Veronica Nacci, Ahmet Nazligul, Alina Negrea, Yeke Ni, Adair Nicolson, Kudakwashe Nyandoro, Zhiyong Pan, Monik Panchal, Anand Patel, Mehzabin Patel, Mikesh Patel, Helena Philpott, Wiktorina Piorkowska, Melis Pisiren, Clarissa Ponan, Daniel Ponsford, Tom Pope, Jay Pritchard, Premrudee Promdet, Mikhail Pumpianskii, Chengwu Qiu, Warda Rahim, Alexis Ralli, Cesar Reyes, Adrien Richard, Valerie Ries, Marwa Rizk, Alexia Rottensteiner, Ethan Rubinstein, Antonio Ruiz Gonzalez, Intisar Salah, Luigia Salerno, Matthew Salinger, Mustafa Sener, Usman Shabbir, Yiana Shakespeare, Andre Shamsabadi, Fengyuan Shan, Ju Hun Shin, Daniel Silva Nunes, Miguel Sipin, Rachael Smith, Belen Sola Barrado, Kieran Spooner, Sriluxmi Srimuruganathan, Alexandria Sterling, Sebastian Stockenhuber, James Strachan, Daniel Sykes, Peter Szijj, Rachel Szpara, Sukhpreet Talewar, Yeshe Tan, Alex Tanner, Roisin Tapley, Omri Tau, Benjamin Thair, Ioanna Thanasi, Anshu Thapa, Benji Thoma, Felix Thompson, Harry Tinker, Kevin To, Thierry Tran, Manish Trivedi, Max Trouton, Ryan Trueman, Jone-Him Tsang, Viliyana Tsanova, Urvashi Vyas, Oliver Walker, Archie Wall, Guanyu Wang, Mingyue Wang, Tianlei Wang, Yiyu Wang, Yu Wang, Catherine Webley, Runzhe Wei, Connor Wells, Megan Westwood, William Whitehouse, Oscar Williams, Joe Willis, Isobel Wilson, Thibaut Wohrer, Ke Wu, Xueming Xia, Zongda Xing, Siyu Xiong, Yijie Xu, Manni Yang, Yuting Yao, Jia'Er Ye, Meltem Yilmaz, Arthur Youd, Jiangdong Yu, Yu Yuan, Anham Zafar, Jichao Zhang, Lina Zhang, Liquan Zhang, Xiangyu Zhang, Xinyue Zhang, Donglei Zhao, Fangjia Zhao, Pinyi Zhao, Siyu Zhao, Yanbo Zhao, Yining Zhao, Yansheng Zhou, Ye Zhou, Lei Zhu, Yiyun Zhu

## Professional Services

#### Computing Officers

D. Ladd  
F. Otto  
L. Willoughby

#### Senior Electronics Officer

T. Bernard

#### EM Technician

S. Firth

#### Glassblower

J. Cowley

#### Instrument Workshop Technician

T. Bridges

#### Chemistry Teaching Laboratories Manager Co-ordinator

A. Philcox

#### Mass Spectrometry Manager

K. Karu

#### Safety Officer

R. Wilson

#### Teaching Laboratory Operations Manager/Technical Safety Officer

C. Medley

#### Buildings/Technical Services Manager

J. Nolan

#### Teaching Laboratory Technicians

N. Bagha  
C. Gacki  
L. Nunar  
H. Shalloe  
M. Towner  
D. Webb  
H. Wong

#### Workshop Technician

A. Delbusso  
S. Edwards

## Administrative Staff

#### Assistant Teaching & Learning Administrator

H. Ambrose-Wilson

#### Assistant Finance Administrator

N. Smith

#### Crystal Structure Prediction Group Manager

L. Price

#### Departmental Manager

R. Wilkinson

#### Deputy Departmental Manager

Y. Moscou

#### Senior HR Officer

N. Phillips

#### Senior Finance Officer

L. Mulcahy

#### Chemistry Goods Manager

T. Field

#### HR Administrator

H. Dansey

#### Project Manager & Scientific Administrator

X. Gu  
E. Lumley

#### Senior Research Administration Officer

D. Underwood

#### Research Administration Officer

E. Buonaura

#### Postgraduate Teaching & Learning Administrator

M. Seetul

#### Undergraduate Teaching & Learning Administrator

M. Nolan

#### Senior Teaching & Learning Postgraduate Administrator

J. Butorac

#### Senior Teaching & Learning Undergraduate Administrator

M. Kelly

#### EA to Head of Department

L. McSeveny

## Emeritus Staff

J.E. Anderson  
A.G. Davies  
A. Deeming  
J.R.G. Evans  
C.R. Ganellin  
P.J. Garratt  
W. Motherwell  
F. Pearce  
J.H. Ridd  
B. Roberts  
P. Smith  
D.A. Tocher  
S. Walmsley



---

## UCL Chemistry

Christopher Ingold Building  
20 Gordon Square  
London WC1H 0AJ

[ucl.ac.uk/chemistry/](https://ucl.ac.uk/chemistry/)

Twitter <https://twitter.com/UCLChemistry>

Facebook <https://www.facebook.com/UCLChemistry/>

Instagram: <https://www.instagram.com/ucl.chemistry/?hl=en>