

UCL Chemistry NEWSLETTER

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Many thanks go to Louise McSeveny, for organising this years newsletter and to Tracy Hankey at UCL Digital Media for her help.

We hope this newsletter gives a flavour of the exciting chemistry and family atmosphere achieved in the department.

It is not an exhaustive document but can provide a number of contact points to the wide variety of activity that occurs in the department.

Introduction by Head of Department



I am feeling very relaxed as I start writing this welcome having just returned from my honeymoon in Croatia after getting married in August! Being able to unwind after another busy year in the chemistry department, many highlights of which are included in this newsletter, was greatly appreciated. We were pleased to see that UCL Chemistry moved up 11 places to 30th in the QS world university rankings by subject (from 41st in 2018). This was one of the biggest uplifts of any subject at UCL and puts us 4th in UK.

This academic year Professor Xiao Guo moved to the Department of Chemistry, University of Hong Kong after 11 years here at UCL. Farzana Hassain (Departmental Administrative Assistant) moved to a new role in Professor Jawwad Darr's group. We welcomed Dr Yang Xu from the

Technische Universitat Ilmenau as a Lecturer in Electrochemical Energy Storage, Dr Cally Haynes from University of Cambridge as a Lecturer in Organic Chemistry and Dr Anna Regoutz from Imperial College as a Lecturer in Materials Chemistry. In addition, Dr Adam Clancy and Dr Gi-Byoung Hwang will both be starting Ramsay Trust Fellowships in the department. We also welcomed Hannah Shalloe as our first Apprentice Technician, Helena Wong who has started as a Chemistry Teaching Laboratory Technician, Thom Dixon as our new Teaching and Learning (Student Lifecycle) administrator, Angelo Delbusso as our Workshop Technician and Malgorzata Puchnarewicz who has joined us as maternity cover for the mass spec facility. Louise McSeveny is now with us permanently as my Executive Assistant, while Nicola Philips on returning from maternity leave has moved to a new position as the departmental Senior HR Administrator.

There have been a number of awards within the department. Two members of the department received awards from the Royal Society of Chemistry. Dr Matt Powner has been awarded the Harrison-Meldola Memorial Prize and I received the Applied Inorganic Chemistry award. Four members of the department were elected to membership of the Academia Europea – Professor Ivan Parkin, Professor Sally Price, Professor Peter Coveney and Professor Paul McMillan. Martyn Towner (Natural Sciences Laboratory Technician based in the Chemistry Department) received a UCL Education Award (Individual) for his outstanding contribution to enhancing and supporting student learning in undergraduate laboratories in the Department of Chemistry. Dr Jadranka Butorac (Senior Teaching & Learning Postgraduate Administrator) received a BEAMS Professional Services Award for giving our students the best support, facilities and opportunities.

Yet again the department had an excellent intake with over 110 students taking one year MSc and MRes degrees in the department. Undergraduate and PhD admissions were also very strong with record numbers of UG students. We have been pleased to be able to invest in new equipment this year including a new High Resolution UPLC-Q-Exactive Orbitrap Mass Spectrometer System, an X-ray Fluorescence Spectrometer, a fluorimeter with NIR capability, a NanoDrop OneC Spectrophotometer and various battery testing facilities to support the Faraday Challenge. Upgrades to the 3rd floor synthetic laboratories continue and we are excited about a major investment by UCL to develop a Laser Science Centre in the basement of the Christopher Ingold Building.

I hope to see many of you at the Annual Lab Dinner in November.

Best wishes

Professor Claire Carmalt

New Appointments

Academic Appointments



Yang Xu Lecturer in Electrochemical **Energy Storage**

Before joining UCL in April 2019, Yang was a Senior Scientist and Group Leader at the Technical University of Ilmenau in Germany (2013-2019) and a Postdoctoral Research Associate

at the University of Alberta in Canada (2012-2013) and Boston College in USA (2011-2012). He received his PhD in Chemistry in 2011 from the University of Science and Technology of China, under the supervision of Professor Yi Xie.

Yang's research focus is electrochemical energy storage technologies with a special interest in rechargeable Sodium- and potassium-ion batteries. Current research within the group focuses on discovering new electrode materials, designing electrode architectures, and understanding the defect structure-battery performance relationship, particularly at local atomic and nanometric scales, as well as investigating solid-liquid/solid-solid interfaces towards local electrochemical reactivity in a battery material system. Furthermore, the group has an increasing interest in exploiting new cell chemistries and the underlying electrochemical mechanisms.



Cally J.E. Haynes Lecturer in Organic Chemistry / Chemical Biology

Before joining UCL in June 2019, Cally was a Postdoctoral Research Associate at the University of Cambridge (2015-2019). She completed her PhD under the supervision of Professor

Philip Gale at the University of Southampton (2009-2011), where she was also awarded an EPSRC Doctoral Prize Fellowship (2011-2012) and worked as a PDRA until 2013. She also worked as a Publishing Editor at the Royal Society of Chemistry, contributing to the production of journals including ChemComm, Chemical Science and ChemSocRev from 2013–2015.

Cally's research interests are in supramolecular chemistry, targeting the development of small molecule probes to perform new functions inside lipid bilayers for biomedical applications. This will involve generating fundamental knowledge on predicting and controlling the membrane binding, partitioning and localisation of small molecules, which will in turn enable precise regulation of their delivery and function. The applications of this work will include producing simple synthetic mimics to replicate the action of natural occurring membranebound proteins and establishing the knock-on effects of introducing these mimics into cellular systems. Other goals will be the application of controlled membranecrossing and partitioning events to mediate the selective delivery and localisation of diagnostic and imaging agents.



Anna Regoutz Lecturer in Materials Chemistry

Anna joined the department in July 2019 as a Lecturer in Materials Chemistry. She is a CAMS-UK Fellow and holds a Visiting Scientist position at Diamond Light Source. Before

joining UCL Anna was an Imperial College Research Fellow (2017-19) and Postdoctoral Research Associate (2015-17) at Imperial College London and a Research Fellow at the University of Southampton (2013-14). She received her PhD in Inorganic Chemistry from the University of Oxford in 2014, where she worked under the supervision of Professor Russell Egdell.

Anna's research focus lies on bulk, thin film, and nano materials for application in devices, including power and flexible electronics, photovoltaics, and biosensors. Her interests include novel growth methods for high quality thin films, nanostructured layers, and nanostructures of inorganic materials with a focus on metal oxides. She works on developing and advancing X-ray spectroscopy methods for bulk materials, surfaces, and interfaces in electronic devices. She concentrates on using and developing both laboratory- and synchrotronbased spectroscopic methods to study in particular the electronic structure in oxide heterostructures. Anna uses her combined expertise in deposition and characterisation of these materials to understand and tune the materials' electronic and optical characteristics to ultimately improve existing device concepts and develop novel device applications.

Promotions

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



Mike Porter
Promoted to Professor of
Organic Chemistry



Matt Powner
Promoted to Professor of
Organic Chemistry



Daren Caruana
Promoted to Professor of
Physical Chemistry



Vijay Chudasama
Promoted to Professor of
Organic Chemistry and
Chemical Biology



Rob Palgrave
Promoted to Professor of
Inorganic and Materials
Chemistry



Tracey Clarke
Promoted to Associate
Professor



Vicky Hilborne
Promoted to Senior Teaching
Fellow

Ramsay Fellows



Adam Clancy Ramsay Fellow

Adam completed his PhD at Imperial College London in 2016 in carbon nanotube composites under Professor Milo Shaffer, before being awarded an EPSRC Doctoral Prize Fellowship to continue his work into nanotube

processing. He subsequently moved to UCL in 2017, originally joining the Institute for Materials Discovery, working on icephobic materials, before returning to nanocarbons when joining UCL's Chemistry Department under Professor Paul McMillan, developing graphene-based fuel cells. As a Ramsay Fellow, he is investigating the solution processing of 2D nanomaterials for optoelectronic and energy storage applications.



Gi Byoung Hwang Ramsay Fellow

Gi obtained his Master's degree from Konkuk University (South Korea). After working at the Korea Institute of Science and Technology (KIST), he joined Professor Ivan P Parkin's group and graduated from UCL with a PhD

in 2018 with his thesis on white light activated bactericidal surfaces. He is currently working as a Postdoctoral Research Associate under supervision of Ivan P Parkin on Manufacturing Advanced Functional Materials. In 2019, Gi obtained a Ramsay Memorial Fellowship which he will start at UCL at January 2020.

Royal Society of Chemistry Awards

Professor Claire Carmalt was awarded the Royal Society of Chemistry Applied Inorganic Chemistry Award for 2019.

Claire was recognised for her outstanding contributions to the synthesis of inorganic CVD precursors and the development of superhydrophobic paint.



Claire's group works on developing robust water repellent materials that can be combined with different adhesives to create "self-cleaning" surfaces, such that water droplets are able to roll over the surface, picking up dirt, viruses and bacteria along the way. The material addresses one of the biggest challenges for the widespread application of self-cleaning surfaces by finding a way to make them tough enough to withstand everyday damage. Research in the group also investigates the synthesis of novel molecular precursors and deposition of films using chemical vapour or spray deposition.

Professor Carmalt said: "I was delighted to find out that I had been awarded the 2019 Applied Inorganic Chemistry Award. Research in my group over the years has focused on developing new materials and investigating how best to use them to improve our daily lives. This award for industrially focused research is a great recognition of the hard work not just from me but from my team and collaborators."

Congratulations to

Prof. Ivan Parkin, Prof. Sally Price, Prof. Peter Coveney and Prof. Paul McMillan who have all been elected to membership of the Academia Europea.

Prof. Claire Carmalt who has been elected as Fellow of the European Academy of Sciences.

Congratulations to Thibault Gendron

at UCL Radio-chemistry and UCL GMP Facility for winning the Royal Society of Chemistry Radiochemistry Group Young Researcher's Award for his work on dibenzothiophene sulfonium salts as leaving groups for 18F aromatic fluorination.



Dr Matthew Powner is the 2019 recipient of the Royal Society of Chemistry's Harrison-Meldola Memorial Prize, awarded for the most meritorious and promising original investigations in chemistry and published results of those investigations.

Matt is awarded for pioneering investigations into prebiotic synthesis, which illuminate key conceptual steps in the origin of life.

The origin of life is one of the great unsolved problems of science. Resolving this problem requires answers to a wide range of questions concerning the underlying prebiotic chemistry, the assembly of the first cells, the advent of Darwinian evolution, and the planetary context of the origins of life.

The Powner group develops new reactions [1-4] and physicochemical methods [5] that can shed light on the process that led to the origin of life on Earth. The group and their collaborators have developed a new modus operandi to investigate the origins of life through the application of 'Systems chemistry'. Rather than attributing functional importance to any one class of metabolite or to one specific environmental niche, concomitant analyses of the chemical constituents of life, their biochemical activation towards macromolecular assembly and the planetary history of the Earth are being undertaken to elucidate the origins of life.

- Canavelli, P., Islam, S. & Powner, M.W. Peptide ligation by chemoselective aminonitrile coupling in water. Nature, (2019).
- 2. Roberts, S.J. et al. Nat. Commun. 2018, 9, 4073.
- 3. Fernandez Garcia, C.A., Grefenstette, N.M. & Powner, M.W. Chem. Commun. 2018, 54, 4850–4853.
- Coggins, A.J. & Powner, M.W. Nat. Chem. 2017, 9, 310–317.
- Islam, S., Bucar, D.K. & Powner, M.W. Nat. Chem. 2017, 9, 584–589.

Congratulations to Jadranka Butorac

Senior Teaching and Learning Postgraduate Administrator who received the BEAMS Professional Services Award for giving our students the best support.

Congratulations to Alex Ganose and Guanjie He

who were jointly awarded the MAPS 2018 Faculty Postgraduate Research Prize for the exceptional quality of their PhD theses and publications in Chemistry.

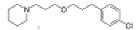
RSC-BMCS Hall of Fame and Medal 2018

Professor C. R. Ganellin

Professor Robin Ganellin received his medal and framed certificate on becoming the inaugural inductee into the BMCS-RSC Hall of Fame (Biological and Medicinal Chemistry Sector of the Royal Society of Chemistry) on March 13 at the Mastering Medicinal Chemistry meeting held at Lilly, Erl Manor, Windlesham, and he lectured on "Discovery of Pitolisant, the first histamine H3-receptor inverse agonist/antagonist for treating narcolepsy".

A new medicine for treating narcolepsy, WakixTM is the result of a collaboration between medicinal chemists, Prof. Robin Ganellin (UCL) and Prof. Walter Schunack (Free University of Berlin), with Prof. Jean-Charles Schwartz (a neurobiologist at an INSERM laboratory in Paris) and Dr. Jeanne-Marie Lecomte who headed a small pharmaceutical company, Bioprojet-Biotech in Rennes and Paris.

The collaboration has produced the compound known by the International Nonproprietary Name, **pitolisant**, 1-{3-[3-(4-chlorophenyl)propoxy]propyl}piperidine hydrochloride (**Wakix**).





The histamine H3 receptor has a marked constitutive activity and pitolisant is a potent inverse agonist/antagonist. Since pitolisant reverses the constitutive activity, it means that pitolisant can put a brake on histamine release at the level where histamine would otherwise inhibit transmission in histaminergic neurons.

Wakix is the first histamine H3-receptor inverse agonist to be taken through all of the preclinical and clinical phases and it has been demonstrated to be effective in treating all major symptoms of narcolepsy. It is a first-in-class medicine that acts on histamine H3 auto-receptors in the brain.

This leads to increased histamine transmission in the brain thereby enhancing wakefulness and alertness and decreases cataplexies and hallucinations in patients with narcolepsy.

It has received marketing authorisation from the European Medicines Agency for treating narcolepsy, with or without cataplexy, in 2016. Wakix was accepted by NICE for the UK in 2017 and received fast track examination from the FDA in the USA in 2018. It has also become on the REF impact case studies for our chemistry department.



Image: Prof. Robin Ganellin receiving his award

Provost Education Awards 2019



Martyn Towner, a member of the Natural Science teaching lab, team is this year's recipient of the UCL Provost Education Award. These awards recognise staff making outstanding contributions to the learning experience and success of our students.

Martyn is one of the Teaching Lab Technicians based in the chemistry department, managing both the thirdyear chemistry undergraduate lab course and the MSc in Applied Analytical Chemistry. He has played an essential part in enhancing the student experience and is a source of outstanding support for the department.

Alexa Marroquin, Chemistry's undergraduate student representative has received the **Faculty Academic Rep of the Year** award for the MAPS Faculty. Alexa has collected vast amounts of student feedback and has endeavoured to talk to staff about issues that affect the students in her department.

The Student Academic Representatives scheme is managed by Students' Union UCL and during this academic year, 1,600 Academic Reps worked across UCL, sitting on committees at programme, faculty and university level, where they act as the voice of students.

EDI Committee Newsletter

Who are we?



We are the Equalities, Diversity and Inclusion Committee. We meet monthly and work proactively within the department to embed equality and diversity practices.



How to get involved

If you would like to become a member of the working committee, please visit our website and complete an expression of interest form.

Link: https://www.ucl.ac.uk/chemistry/edi-team

Letter from the Chair



It has been a pleasure to work with the EDI team this year. It's been a busy year with the introduction of the coffee mornings, our first thesis writing workshop, a new checklist to provide greater clarity in terms of health/safety when pregnant, the new website and twitter account, various talks/events (e.g. Mental Health & Wellbeing in the Workplace, Carers talk), appointment of our new PDRA tutor, overseeing how our Department's case study model for promotion awareness is being implemented at Faculty level, use of positive action to encourage equal opportunity, etc. We also have new screens to be put up in the department in the coming months, a careers event in early September and a new mentoring scheme to look forward to. I would like to take the opportunity to thank the team for all their hard work - all members have contributed and deserve a lot of credit with the appointment of Nicola Phillips as Deputy Chair & EDI Officer being a great addition.

Professor Vijay Chudasama Chair of EDI Committee 2018/19

LGBTQ+

Hey there! My name's **Jamie Riley** and my role in the Department is mixed between doing super cool research with ultrafast lasers (alas, I work near 300 K) and teaching undergraduate physical chemistry courses. But one of the most exciting aspects of my job is being a member of the departmental Equality, Diversity and Inclusion (EDI) committee – specifically, championing LGBTQ+ issues both in the workplace and with your university experience as a student. Why I love this so much? Well, we're really at the forefront of pushing boundaries and coming up with innovative ideas to challenge and change the status quo. Why's this important? Simple. Representation matters! As much as some people might not like to admit it, or might save the reservation for the humanities, science is creative. Only your unique experiences, personality and ambitions are what can drive the process for new concepts and creative thought. We as a Department then must ask, how do we create an environment and

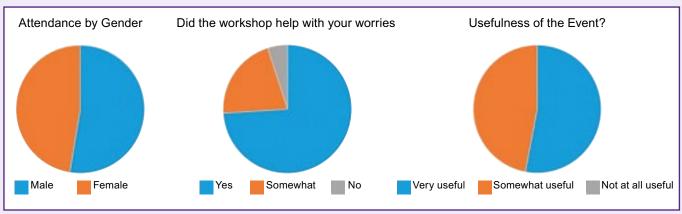


safe-space that allows for this? The answer really is simple, people, regardless of who they are, must feel comfortable to truly express themselves without any reservations, fear of discrimination or onset of inappropriate behaviour. Unapologetically and unashamedly themselves. One of our most recent feats has been the introduction of **Friends of Out@UCL** and Out@UCL stickers being provided to all members of staff within the Department. A simple item, such as a sticker, allows for greater visibility to LGBTQ+ people that can be valuably reassuring. We're pleased to see this has already been taken up by many members of the Department, and I must say, the building is looking ever the prettier for it. Also, coming this academic term will be the creation of a new LGBTQ+ network within the Department. This will be open to absolutely anyone, regardless of how you identify, and aims to be a relaxed and friendly setting where people can chat, meet new people, get their concerns and ideas out, and we'll even be arranging fun activities! Details to come, so make sure you keep up to date with all our exciting news and ideas by following us on twitter @EDIUCL – see you around!

Thesis Writing Workshop

We are pleased to announce that our department's first thesis workshop was a great success, with overwhelmingly positive feedback. The aim of the workshop was to improve and increase support for PhD students when entering and considering the writing up stage of their doctorate. Based on our follow-up survey results, we achieved this aim, and attendees reported a highly positive experience at the workshop. However, the good work should not stop there, and the EDI committee would love to hear any more thoughts and ideas that members of our community might have to create an even more supportive environment for our department and improve on the steps that we have already made. The thesis writing workshop will be making an annual appearance, so watch this space for those improvements. Image: Thesis Writing Workshop 2019





EDI Events

Coffee Mornings

We hold weekly coffee mornings on **Wednesdays** from **10.30am** – **11.30am** in the Nyholm Room. This is an informal coffee open to all staff to socialise and network. Please feel free to pop along, we only ask you bring your own mug!

19th November 2019

International Men's Day: Join us in celebrating the positive value the men in Chemistry bring to the world, their families and communities.

4th December 2019

International Day of People with Disabilities (3rd December): To mark IDPWD, the department is inviting the Chair of the Enable Network to the coffee morning to explore relevant topics for disabled staff.

March 2020

The EDI Team are currently putting together a schedule of events to celebrate **International Women's Day**. We will be looking at the superstar women in Chemistry, what kick started their careers and what advice they give to others wishing to pursue an academic career.

If you have any topics you would like the committee to explore, please do get in touch with us.

Contact Us

Website: https://www.ucl.ac.uk/chemistry/equality-diversity-inclusion-edi

Email: chem.edi@ucl.ac.uk
Twitter: @UCLChemEDI



It's start of term. Today we celebrate the 75th anniversary of our colleague Alwyn Davies arriving @ucl as an undergraduate. He's been a student, a prof, a Head of Dept, a great teacher, and eminent researcher. Above all he's been a friend and a mentor to many of us.





Chemistry Department staff at this year's graduation ceremony, Royal Festival Hall, 4 September Left to right: Mr Mike Kelly, Dr Krešo Bučar, Dr Dewi Lewis, Prof. Ivan Parkin, Prof. Claire Carmalt, Dr Martijn Zwijnenburg, Dr Stephen Potts, Prof. Katherine Holt, Prof. Chris Blackman, Prof Tom Sheppard, Prof. David Scanlon, Dr Gemma-Louise Davies, Prof. Daren Caruana

2018 – 2019 PRIZE WINNERS

We would like to congratulate the following prize winners:

Undergraduate Prize Winners

TERESA INSINNA

CK Ingold Prize

For Excellence in Undergraduate Performance

ISOBEL DUDLEY

CK Ingold Prize

For Excellence in Undergraduate Performance

SADIA BEGUM

CK Ingold Prize

For Excellence in Undergraduate Performance

CONNIE YANG

CK Ingold Prize

For Excellence in Undergraduate Performance

HARRY LI

CK Ingold Prize

For Excellence in Undergraduate Performance

KRISTINA KOSTADINOVA

CK Ingold Prize

For Excellence in Undergraduate Performance

KATARINA BRLEC

Neil Sharp Prize

For Excellence in Theoretical (including Computational) Chemistry

SORINA IACOBAN

Parke Davis Prize

For Excellence in Medicinal Chemistry

JORIS SIMAITIS

Harry Poole Prize

For Excellence in Physical Chemistry

ASHLEIGH KIRS

Ronald Nyholm Prize

For Excellence in Inorganic Chemistry

ROSALIND STRANG

Charles Vernon Prize

For Excellence in Biological Chemistry

YASSIN HJIEJ ANDALOUSSI

Franz Sondheimer Prize

For Excellence in Organic Chemistry

PhD Prize Winners

KATARINA BRLEC

Supervisor: David Scanlon Ronald Gillespie Prize

 For the best graduate starting a PhD in Inorganic/ Materials Chemistry

NEHAAL AHMED

Supervisor: Vijay Chudasama

Tuffnell scholarship

- For the best graduate progressing to the research school

Second Year PhD Poster prizes

We are pleased prizes were awarded for the best 2nd Year PhD poster to the following students:

Computational Chemistry: Alexander Gheorghiu

Supervisor: Peter Coveney

Organic Chemistry: William Whitehouse

Supervisor: Stefan Howorka

Inorganic Chemistry: Kristian Mears

Supervisor: Claire Carmalt

Physical Chemistry: Roshni Malde

Supervisor: Jamie Baker

Rothwell Prize for best poster in synthetic inorganic chemistry: Helena Philpott

Supervisor: Helen Hailes

Chemistry Prizes

On the 26 June 2019 Professor Claire Carmalt (Head of Department) congratulated the following final year PhD students who were awarded prizes for the best presentation in each of the major research areas of Organic/Medicinal, Inorganic/Materials, Computational and Physical Chemistry, as assessed by a committee.

STUDENT HIGHLIGHTS AND NEWS



Sebastian receives his Catlow Prize from Prof. Claire Carmalt

SEBASTIAN DIXON

Catlow Prize

Supervisors: Ivan Parkin and

Claire Carmalt

Best PhD presentation in Inorganic Chemistry for his presentation entitled: Understanding mobility trends in transition metal doped In2O3:M (M = Mo, Hf, Zr, Sn

Robert receives his Catlow Prize from Prof. Claire Carmalt

ROBERT SINCLAIR

Catlow Prize

Supervisor: Peter Coveney

Best PhD presentation in Computational Chemistry for his presentation entitled: Multiscale Modelling of Graphene's **Mechanical Properties**



Catherine receives her Ewing Prize from Prof. Claire Carmalt

CATHERINE HIGGINS

Ewing Prize

Supervisor: Steve Price

Best PhD presentation in Physical Chemistry for her presentation entitled: The Interactions and Reactions of Small Molecules on Astrochemically Relevant

Surfaces



Peter receives his Davies Prize from Prof. Claire Carmalt

PETER SEAVILL

Davies Prize

Supervisors: Jon Wilden and

Katherine Holt

Best PhD presentation in Organic Chemistry for his presentation entitled: Utilising Copper for Methodological Advancements in Electro-Organic Synthesis

Honourable mention to runners up:

Inorganic chemistry: Jian Guo

Physical Chemistry - Gabriele Marchello

Organic Chemistry - Jianxiong Zhao & Andre Shamsabadi

Graduating Students

MIREN AGOTE ARAN

PhD Chemistry

Supervisor: Andrew Beale

ABDULLAH ALOTAIBI

PhD Chemistry

Supervisor: Ivan Parkin

KATHRYN ASHE

PhD Chemistry

Supervisor: Matthew Powner

DUSTIN BAUER

PhD Chemistry

Supervisor: Jawwad Darr

GAVIN BELL

PhD Chemistry

Supervisor: Ivan Parkin

GIULIA BOUCHER

ENGD

Supervisor: Dario Alfe

JACOB CHAPMAN

ENGD

Supervisor: Dorothy Duffy

ADAM CLARK

ENGD

Supervisor: Gopinathan Sankar

MERINA CORPINOT

PhD Chemistry

Supervisor: Dejan-Kresimir Bucar

ELEANOR DANN

PhD Chemistry

Supervisor: Richard Catlow

DONATO DECAROLIS

PhD Chemistry

Supervisor: Andrew Beale

RACHEL FLETCHER

PhD Chemistry

Supervisor: Ben Slater

CALLUM FODEN

PhD Chemistry

Supervisor: Thomas Sheppard

ALEX GANOSE

ENGD

Supervisor: David Scanlon

FELICITY GOSSAN

PhD Chemistry

Supervisor: Stephen Price

THEODORE HAYES

PhD Chemistry

Supervisor: Jonathan Wilden

LUCA IUZZOLINO

ENGD

Supervisor: Sarah Price

GALVIN KHARA

ENGD

Supervisor: Dorothy Duffy

LEONA LEIPOLD

PhD Chemistry

Supervisor: Helen Hailes

YAOMIN LI

PhD Chemistry

Supervisor: Christopher Blackman

EVA LIATSI DOUVITSA

PhD Chemistry

Supervisor: Giuseppe Battaglia

KIT MCCOLL

PhD Chemistry

Supervisor: Furio Cora

IMMAD NADEEM

ENGD

Supervisor: Geoff Thornton

JOSEPH NEWCOMBE

PhD Chemistry

Supervisor: Thomas Sheppard/Alethea Tabor

HA NGUYEN

PhD Chemistry

Supervisor: Stefan Howorka

STEVEN PACMAN

PhD Chemistry

Supervisor: James Anderson

ROSSELLA PROMONTORIO

PhD Chemistry

Supervisor: Charles Marson

ENCARNA PUCHETA MARTINEZ

PhD Chemistry

Supervisor: Francesco Gervasio

GENEVIEVE PUGH

PhD Chemistry

Supervisor: Stefan Howorka

MIGUEL QUESADA GONZALEZ

PhD Chemistry

Supervisors: Ivan Parkin and Claire Carmalt

LISA RICHARDS

PhD Chemistry

Supervisor: Richard Catlow

SAMUEL ROBERTS

PhD Chemistry

Supervisor: Matthew Powner

CHRISTOPHER SAVORY

PhD Chemistry

Supervisor: David Scanlon

HARRIET STORY

PhD Chemistry

Supervisor: Alethea Tabor

AISHA SYED

PhD Chemistry

Supervisor: James Anderson

FELICITY TAYLOR

PhD Chemistry

Supervisor: Richard Catlow

DIANA TEIXEIRA GOMEZ

PhD Chemistry

Supervisor: Robert Palgrave

OLIVER WARE

PhD Chemistry

Supervisor: James Anderson

TINGTING ZHAO

PhD Chemistry

Supervisor: Xiao Guo

UCL Chemistry Outreach



Deega & Desmond



Lego Spectrometer



Bright pink NOx



Collecting

In additional to welcoming 1000s of students and teachers to the department for outreach days, our undergrad students have been involved in two very exciting projects.

Deeqa and Desmond are both about to start their third year in Chemistry and were enlisted by Prof. Andrea Sella to help run some exciting projects over summer with two local schools. The idea started as an opportunity to provide important outreach to schools on what chemistry has to offer and to break down stereotypes of what a scientist may look like.

The first project was to highlight air pollution working with two local schools. The first was Highbury Grove, a secondary school Academy in the City of London. The second was a referral centre for excluded students in south London, which we believe sends a positive message to those pupils who are on the margins of mainstream education that they have not been abandoned. Deeqa and Desmond took their knowledge from first year labs to collect NOx - nitrogen oxides that contributes to the formation of smog and acid rain, but also plays a role in affecting tropospheric ozone - an important region protecting us from harmful UV radiation.

Deeqa and Desmond brought kit from our labs, helped the students assemble it, and got them to make a cool looking lego spectrometer. The students were asked to select locations around London to test for NOx, and work began on analysing concentrations from these different locations.

By using a known stock solution, the NOx formed a bright pink colour when in high concentrations - bringing the science to life with a colour scale of how bad air pollution is in certain areas.

The second project saw Deeqa and Desmond team up with Thames 21 (who clean the Thames) and Helen Czerski, an oceans physicist, to start work on the Thames Plastic project: understanding all the different types (and there are many) of plastic that come into our river.



Cleaning

One hundred randomly selected samples were chosen from the Thames, cleaned and subjected to IR spectroscopy, which reveals key signatures allowing for the identification of the plastic, to then begin work on creating a database on all the different plastic types. They even noted any labels left on the plastics to get an idea of where the plastic might have come from. The department is now providing Raman spectroscopy training, to help gain a greater insight into the exact composition of these plastics from structural fingerprints.

Both Deeqa and Desmond both said they have really appreciated the opportunity to get this experience and enjoyed working with pupils to bring chemistry to life.

Congratulations to students in Prof. Helen Fielding's group Anand Patel & Alice Henley.

Anand won the presentation prize for his talk on the synthesis and anion photoelectron spectroscopy of oxyluciferins at the 1st UK(RSC)-IT Joint Meeting on Photochemistry in Lipari, Italy, 24 – 26 June 2019.

Alice won the RSC Poster Prize at the Faraday Discussion Meeting on Advances in Ion Spectroscopy for her poster titled `New twists on the relaxation dynamics of the photoactive yellow protein chromophore'.

Chemical & Physical Society Annual Report 2018-19

By Dr Stephen Potts, President

The Chemical & Physical Society (CPS) was founded in 1876, which makes it UCL's oldest student-run society! The cornerstone of the CPS is its committee, comprising dedicated and enthusiastic undergraduate students and postgraduate researchers, who organise and run the events. Academic staff sit on the committee as President and Vice-President in mentoring and advisory roles, but it was safe to say that, this year, the mentoring was not necessary! The main draws of the CPS are its weekly talks, held on Tuesday evenings during term-time, in addition to social events and, of course, the coveted colour-changing CPS mug.

This year marked the 143rd academic year of the CPS and there certainly seemed to be no sign of it slowing down, with the Ramsay Lecture Theatre being packed out almost every week. This year's programme kicked off with a talk by Prof. Duncan Wass (University of Bristol) on "Directions for Catalysts: Biofuels to Self-Healing Planes", describing how catalysis is employed to create materials from advanced biofuels, such as methanol, to self-healing planes - particularly important when carbonfibre is replacing aluminium in airframes.

We then moved on to "Molecules of Murder" by Dr John Emsley (science writer). The talk, based on his book of the same name, contained lots of useful advice on how to dispatch unwanted people (provided you wanted to get caught). This was John's fourth visit to the CPS; having spoken to us in 1996, 2006 and last year. We'd gladly have him back again, but he'd have to write a new book! The following week's talk took us to the opposite end of the health spectrum; i.e. assessment of public health. In her talk "Urban Water Fingerprinting to Inform of the Environment & Health", Prof. Barbara Kasprzyk-Hordern (University of Bath) introduced us to a cutting-edge approach of waste-water analysis, which gave insight in the general health of the local population and allowed for prediction of health risk.

Continuing on the topic of health, Dr John Marsden (King's College London) gave a fascinating presentation on "Mental Images & Memory Processes as Targets for Cocaine Use", in which he described how observation of cocaine users has led to new insights into how psychological therapies can be adapted to treat addiction. There were some rather uncomfortable videos shown that really hammered home how important effective addiction therapy is.

The following week, we hosted our annual careers event, where speakers with chemistry degrees explained how they got to where they are today. This event was very well attended and promises to be bigger next year! The next talk followed on nicely, as UCL graduate Dr Anna Ploszajski (science communicator) gave an enthusiastic overview of "Smart Materials" and the challenges associated with them, which is why their widespread adoption has been somewhat limited, despite their promising applications.

"Mind Reading and Interpersonal Attraction" was the topic of our next talk by Dr Prof. Barbara Kasprzyk-Hordern Peter Mitchell (University of Nottingham). Peter demonstrated that people are more skilled at mind reading than they might realise and talked about the subtle cues we fingerprinting don't realise we respond to. It was certainly mind-expanding and something I'll be using



The committee signing up new members in September



Dr John Emsley giving his talk on "Molecules of Murder".



giving her talk on water

on colleagues in the future. Sticking with matters of the brain, the following week Prof. Stephen Brickley (Imperial College London) discussed "Age-Related Changes in Synaptic Transmission in Cognitive Design". He described that, rather depressingly, synaptic decline starts in humans in their 20s. However, a greater understanding of this decline has led to improvements in treatment for people suffering from lapses in cognition.

STUDENT HIGHLIGHTS AND NEWS

For our last talk of 2018, we left Earth to hear about "Molecules in Space: Our Astronomical Origins" by Dr Catherine Walsh (University of Leeds). The complex organic molecules that make up life originated from simple molecules, such as H, and CO, nucleating on interstellar ice and asteroids. It was fascinating, eye-opening stuff. Later that week, we said goodbye to the year with our infamous Christmas Quiz. Apparently, the theme tune to "Arthur" is very popular with chemists.

The new year kicked off with Prof. David Nutt (Imperial College London), who is famous for his former governmental role. His talk, "Why We Must Change the Drug Laws to Liberate Research and Treatment", covered how many of the UK's drug laws are based on moral issues rather than scientific evidence. There was a lot of data to back up his claims and it certainly marked an exciting start to 2019!

Dr Lizzy Ostler (University of Brighton) followed on with "Will Red Wine and Chocolate Really Keep You Young and Healthy?", which looked at myths like a glass of red wine a day being good for you (isn't it?). From food to scents, Ruth Mastenbroek (perfumer) gave one of the few talks with an equation as the title: "Perfume = Chemistry + Artistry: An Interactive Talk". She covered the history of perfume and the associated molecules before explaining why the ingredients of perfume are never revealed on products, all while handing round samples. The Ramsay Lecture Theatre has never smelt sweeter!

By far the most popular talk of the term (indeed the year) was "The Science of Climate Change - and What We Can Do About It". Prof. Joanna Haigh (Imperial College London) gave a sobering overview of the current state of the Earth's climate, with clear scientific evidence demonstrating the rise in global temperature and carbon dioxide levels. However, she gave some sound advice on possible solutions to slow down these increases.



terms of what their manufacturers could claim in advertising in "The Rise and Fall (and Rise Again?) of Probiotics". However, she showed evidence that taking care of your gut biome really can benefit your general wellbeing, anticipating a resurgence in their use. This talk was followed by Dr Rebekah Higgitt (University of Kent), whose talk, "The First Prize Medal for Science: The Origin of the Royal Society's Copley Medal", was a fascinating history of the esteemed prize.

From the historical to the modern. Dr Stephen Hilton (University College London) showed that a lot of money could be saved by printing lab equipment and consumables in "3D Printing and its Applications Across Pharmacy and Chemical Synthesis". He went on to show how printing cases for magnetic stirrer bars can beneficially alter catalytic routes in certain chemical reactions. This was followed by a PhD speaker, Cerys Bradley (University College London), whose talk "Measuring the Dark Web" explained how the internet can be exploited for drug use and what is being done to combat it.

The last two weeks of the term turned to alcohol. Prof. Andrew Whiting (Durham University), who also runs the company pHure Gin, talked about "Gin: the People's Tonic". He presented a history of gin before explaining that pHure distils the gin at low pressure so that the lighter volatiles are retained, giving the it a distinct flavour profile. We all had a chance to try it and it was delicious (from what I remember).

Lastly, Dr Stephen Potts (University College London) changed his usual wine-tasting into a talk: "In Vino Veritas (et Moliculis)". He presented 13 molecules that are key aroma and flavour components in wine and described their origins. Although everyone's nostrils were saturated by the end of the presentation, and the department smelled of old cork for the next week, it went down well with everyone (the post-talk wine helped too).

To round off the academic year, the CPS hosted its third Boat Party. Students from all year groups donned their best outfits to party the night away on the Thames and forget about impending exam results.

For more information about the CPS and the talk schedule for the next academic year, please visit www.cpsucl.com. Don't forget to follow us on Facebook, Twitter (@CPSUCL) and Instagram (@cps_ucl), too!



The CPS committee at the annual Chemistry Lab Dinner



Committee members listening to

Spectroscopy and Dynamics Seminars

We have hosted a series of weekly seminars that began in January 2019 and have hosted a diverse group of speakers from the Chemistry department and beyond in the broad field of spectroscopy and dynamics.

In January several research groups within the Department of Chemistry banded together to run the 'SDG seminars' the spectroscopy and dynamics group seminars - based on shared research interest. This includes the groups of Helen Fielding, Stephen Price, Tracey Clarke, Graham Worth and Geoff Thornton, and the organising committee is formed from PhD students and Postdocs from each group.

We organise seminars on a weekly basis during term-time, from within our own groups and from further afield. External speakers have included Dr Artem Bakulin from Imperial College London, Dr Rachel Crespo-Otero from Queen Mary University of London, Prof. Gaetana Laricchia from University College London Physics and Prof. Katherine Holt from University College London as well. Each of these external speakers delivered a talk on their research for the relatively general audience of the SDG and anyone else who saw us advertising in the chemistry weekly newsletter!

Being a spectroscopy and dynamics focussed group does not restrict us in the choice of invited speakers, and we aim to find external speakers who work on the edge of something new – such as Professor Laricchia who gave a delightful and informative talk on positronium scattering from gas-phase molecules. To this effect, we are open to speakers from other aspects of physical chemistry as well. We often head to a local pub after the meeting to talk shop, so the group is a social one as well.

As a student and postdoc led meeting, we encourage everyone to present and chair, particularly the Masters and PhD students. This gives everyone a chance to practise this skill in front of a friendly audience. The environment also functions for getting feedback on new results, to pool our collective experience and understanding.

If anyone is interested in being added to the mailing list, or presenting their own work during the next year, please contact me. It is a welcoming environment designed for perfecting presentations for conferences and provides an opportunity to interest others in your work.

Dr Lily Ellis-Gibbings



ISOBEL WILSON is doing her PhD with Katherine Holt and Mike Porter, won the 'Three Minute Thesis' competition at the MAPS faculty heat in June.

Isobel's talk was about the benefits of using electrochemistry in organic synthesis, such as reducing waste and

toxicity. However, the uptake of this method of synthesis is slow in the organic community. Her research focuses on trying to develop a useful and adaptable electrosyntheic reaction to highlight the benefits of this type of process.



ELEANOR DANN is the recipient of the 2018 Ramsay Medal. After graduating from University of Bristol in 2015, Ellie started her PhD with UCL under the supervision of Professor Richard Catlow and Dr Peter Wells (University of Southampton) in the

Eleanor Dann received her Ramsay Medal from Prof. Claire Carmalt at the 2018 Chemistry Lab Dinner

field of heterogeneous catalysis. Throughout the duration of her PhD, Ellie has been part of the UK Catalysis Hub located at the Research Complex in Harwell. As an industrially funded iCASE student, Ellie has worked closely with Johnson Matthey Technology Centre to provide greater understanding of the heterogeneous catalyst materials for emissions control technology. This has involved designing a new reactor for time-resolved X-ray absorption spectroscopy (XAFS) and diffuse reflectance infrared spectroscopy (DRIFTS) of supported palladium nanoparticle materials during catalytic operation for specific reactions; CO oxidation, selective NH3 oxidation and CH4 oxidation. Over the last three years Ellie has collaborated with beamline scientists at Diamond Light Source, the European Synchrotron Radiation Facility and the Swiss Light Source to make significant advances to the characterisation of supported nanoparticle catalysts, with work published in ACS Chemistry of Materials and Nature Catalysis. Ellie is now writing her thesis titled 'Improving Synchrotron Methods for Advanced Characterisation of Heterogeneous Catalysts', and has ambitions to train as a patent attorney.

2019 CHEMISTRY LAB DINNER

We are pleased to announce that this year's Chemistry Lab Dinner will be taking place on

Friday 22nd November 2019

at the Ambassadors Bloomsbury Hotel

For further details please visit our website: http://www.ucl.ac.uk/chemistry/about-us/chemistry-lab-dinner



This year we are thrilled to announce the Thomas Graham Lecture will be given by Dr Matthew Powner. Matt was born in Wensleydale, North Yorkshire in 1981. He obtained a first class master's degree in chemistry at the University of Manchester (2005), where he was awarded the Royal Society of Chemistry prize, the Degussa award, the Sigma-Aldrich prize, the Glaxo prize, the Eric Braithwaite prize, the Swan prize and the Merck Sharp & Dohme award. He then completed a medicinal chemistry internship at AstraZeneca, Alderley Park, before returning to Manchester to complete his PhD (2009) and a short EPSRC Doctoral Prize post-doctoral fellowship with Prof. John Sutherland FRS. In 2009 he was awarded a

Harvard Research Fellowship to work with Nobel Laureate Prof. Jack Szostak FRS at Massachusetts General Hospital and Harvard Medical School. He returned to the UK in 2011, joining UCL as a Lecturer in the Chemistry Department, where he is currently a Professor of Organic Chemistry and an Investigator of the Simons Foundation Collaboration on the Origins of Life. His research interests centre around chemistry associated with the origin of life and, along with his research group, has made contributions in the areas of nucleic acid and amino acid chemistry, protometabolic networks, ribozymes, lipids, crystal engineering, green chemistry, catalysis and photochemistry. Dr Powner has been awarded various prizes and fellowships in recognition of his research, including the ISSOL Stanley Miller Award (2011), the SET for Britain Roscoe Medal (2012), 1st prize in the Origins of Life Challenge (2012; jointly with Prof. John Sutherland FRS), an EPSRC Early Career Fellowship (2013), a Bürgenstock JPS Fellowship (2015), the Thieme Chemistry Journal Award (2015), a Center for Advanced Studies Fellowship (2016) and the RSC Harrison-Meldola Memorial Prize (2019).



Our after-dinner speech will be given by Ebony-Jewel Rainford-Brent who graduated with a MSci in Chemistry in 2006 and went on to play with the England team that won the 9th ICC Women's Cricket World Cup, the World T20 and Women's Ashes in 2009. Ebony-Jewel was awarded UCL Sportswoman of the Year in March 2007 and was the first Director of Women's Cricket at Surrey County Cricket Club.



Since retiring from sport, Ebony has gone on to a career in the media including becoming a broadcaster and commentator for the flagship BBC programme 'Test Match Special', as well as following her passion for personal development as a Motivational Speaker and Performance Coach.

We have also invited the President of the Chemical and Physical Society, Dr Anna Roffey to give a short speech on the current status of the CPS and how you can get involved. Anna joined the department as Teaching Fellow in 2017.

How to secure your place

We operate on a first come, first served basis and have 80 places available.

The full cost of the evening is £45. For current postgraduate students, a limited number of tickets will be charged at £25. To book your place at this year's event, please complete a booking form (found on the link above) for payment information. All cheques should be made payable to "University College London".

Tickets are non-refundable.

Obituary



Robin Clark 1935 – 2018

Robin Clark, who had been a member of the Department for 60 years, died on December 6, 2018 after a short illness. He was a distinguished physical/inorganic chemist who made major discoveries in the chemistry of the early transition metals, especially of titanium

and vanadium compounds with high coordination numbers, and of mixed valence, linear chain and metal-metal bonded complexes. He was also known for developing techniques of far infrared, Raman and resonance Raman spectroscopy applied to inorganic compounds, including pigments used in artworks and historical artefacts, thereby establishing a basis for verifying their provenance and identifying forgeries.

Robin was born in Rangiora in New Zealand, in 1935, and took a BSc and MSc degree in chemistry at Canterbury University College from 1953 -1958. He started a PhD at Otago University, but his supervisor, W.S. Fyfe moved to Berkeley. Robin then applied to work with Professor Ron Nyholm at UCL: on the toss of a sixpence he decided to accept the offer and after a long journey by boat and train he arrived in the UK on 29 July 1958. He spent all of his subsequent career in the Department, but always remained proud of his New Zealand heritage and kept strong contact with his homeland.

Ron Nyholm was widely seen as being responsible for the renaissance of inorganic chemistry, and the Department was a very lively place with a large contingent of Australian research students and staff who played in the departmental "Australia versus The Rest" cricket game. As a New Zealander, Robin was co-opted on the Australia team. Ron was interested in the chemistry of the transition metal elements and their complexes. Although highly (7- and 8-fold) coordinated complexes were known with Zr and Hf, it was widely believed that these would not form with early transition metals due to steric congestion. However, in his Ph.D. work Robin prepared the 8-coordinate complex

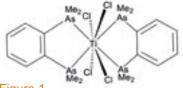


Figure 1

O=0 O=Pt x 226A y 3.13A
Figure 2

[TiCl₄(Diars)₂] between titanium tetrachloride and the diarsine ligand 1,2-C₆H₄(AsMe₂)₂ (Fig. 1), leading to a *Nature* paper.

He was appointed as a lecturer in 1962 and rapidly built up his own research group, using reflectance UV-visible and far-IR spectroscopy to study inorganic compounds and solids. He later developed and applied Raman and resonance Raman techniques in complementary research.

In 1968 Robin published what is still regarded as the definitive monograph on the chemistry of Titanium and Vanadium, followed by volumes on Titanium, Zirconium and Hafnium, and on Vanadium, Niobium and Tantalum, He worked on the chemistry of complexes of Ni(II), Pd(II), Pt(II), V(III), and Cr(III). These compounds are highly air- and moisture-sensitive, and at the time UCL had no capability to handle them. Robin took a Linguaphone refresher course in German and translated a Ph.D. thesis from Jena that contained the necessary information. He then worked with departmental glass blowers to produce equipment that he used to establish the structures by diffraction and spectroscopic methods. Many types of compounds were studied, including metal-metal bonded compounds such as [Mo₂Cl₈]⁴⁻ and [Re₂F₈]²⁻, and the mixed-valence chlorinebridged Pt(II)-Pt(IV) Wolffram's salt (Fig. 2). His work on Ni, Pd and Pt compounds began when he spent time with Harry B. Gray at Columbia University in New York, where the two friends appeared to improve their tennis skills while advancing science. When Harry moved to CalTech in 1965, Robin spent several months replacing him as visiting Associate Professor.

Robin's use of far-IR spectroscopy to study metalligand vibrations in halide and other complexes attracted considerable attention and it established use of the technique for structural characterisation. He later played a leading role in developing laser Raman spectroscopy as part of the University of London Intercollegiate Research Service (ULIRS) that he directed from 1970-73. The first instrument installed at Imperial College had the spectrometer in one room and the laser arrived through a hole in the wall from next door. Later Robin acquired funding for two state of the art Spex spectrometers that he installed at UCL, along with capabilities for multi-wavelength laser excitation. That permitted him to obtain the first Raman spectra of many highly coloured compounds, including pigments that later led to his work on artworks and ancient manuscripts. He soon began to investigate and then develop the technique of resonance Raman spectroscopy, where the interaction between electronic and vibrational transitions as a function of the laser excitation wavelength cause remarkable enhancement of certain Raman-active modes, including observation of extended progressions of overtones leading to analysis of anharmonicity parameters and opto-electronic coupling coefficients. His influential review of the field in Angewandte Chemie in 1986 as well as his editorship of "Advances in Infrared and Raman Spectroscopy" and "Advances in Spectroscopy", and co-authorship

of "Raman Spectroscopy" established Robin as one of the international leaders in the field, and his UCL Raman laboratory based in Chemistry as one of the main centres of activity.

Robin then complemented the Raman instrumentation by acquiring a micro-beam Raman instrument. The microscope could focus the incident laser beam and collect spectra from individual grains and regions within a sample as small as 2-5µm in diameter. Steve Best had joined Robin's group in 1984 to investigate electronic transitions and reaction mechanisms in transition metal complexes, and also developed a spectro-electrochemical cell for in situ studies and control of redox-active species. He received a phone call from UCL History of Art following a newspaper report describing the use of Raman microscopy to identify lapis lazuli, an important pigment. Robin had already worked on ultramarine blue to identify the chromophoric species S2and S3- responsible for the characteristic intense colour. Although initially sceptical because of the possibility that electronic fluorescence could swamp the weak Raman signal, they showed that spectra could be successfully obtained using the microbeam technique. This led to a long and successful collaboration between Robin and library, museum and gallery curators to study and evaluate artworks and historical documents using Raman microspectroscopy. Initially, manuscript fragments for examination were assembled by Mrs Cheryl A. Porter of the History of Art department, and her input became critical for establishing contacts with curators or conservators who would permit laser illumination of their illuminated manuscripts. Later, Robin acquired a more portable Renishaw Raman spectrometer that included a fibre-optic attachment to enable scanning valuable documents in situ at their location. That led to important studies carried out in collaboration with many institutions, particularly the British Library. Robin and his team studied paintings and illuminated letters on over 100 manuscripts from some 25 countries ranging from

Korea, Thailand, India, Persia, Turkey, England, Iceland, and Colorado, and they varied in date from the 13th century BC to the 18th century AD. This included the Lindisfarne gospels ca. 715 AD, three of Gutenberg's printed bibles (1455), and the Vinland map which purported to show a pre-Columbus outline of the North East coast of North America, that their work showed to be a forgery. They also showed that the purported painting by Mark Chagall, dated 1910, of a *Nude Woman Reclining*, contained pigments which were not available until the 1930s. This work was dramatised on the BBC's programme *Fake or Fortune* in January 2014.

As Head of the Chemistry Department from 1989-1999. Robin took office at a difficult time when undergraduate numbers were low, and the Department ran at a large annual deficit according to a financial model that measured space required for teaching and research that were large for an experimentally-based discipline, against student numbers. Robin immediately set up a recruitment committee with clear goals to attract new students and the intake numbers improved. Ten staff vacancies occurred during his headship (1989-1999) and each time Robin won a battle with the Provost to be allowed to fill those positions, and excellent appointments were made. He also fostered cooperation with other departments in the science faculties and, with Peter Day, persuaded the Provost to agree that the Royal Institution and the Department should join forces: RI students could now register for joint PhD projects with access to EPSRC grants, and their numbers could be included in the RAE grading of Chemistry Departments. The RAE score rose to 4 in 1989 and later achieved 5* in 2001.

Robin was elected a Fellow of the Royal Society in 1990 and was made a Companion of the New Zealand Order of Merit (CNZM) in 2004 and won a large number of other awards including the Royal Society's Bakerian Lectureship and the Royal Society of Chemistry's Liversidge Lectureship.

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.

From Kerala to London: using UCL's records to rediscover a father's story

When Gopal Krishnan contacted UCL Alumni to help retrace his father's path to UCL, he had the chance to see his father's old student records and visit with staff and tour the Chemistry Department.

Many look to their family history for insights into their own identity. UCL was thrilled to help one man do just that during a visit to the UK from his home in India.

Gopal Krishnan is a mentor and advisor for Ayurveda Wellness Centres and Hospitals in Kerala. He recently came to the UK with his wife, Latika, to visit their daughter. While here, he wanted to find out more about his father, and role model, Krishnan Gopalan Unnithan (BSc Chemistry, 1934).

Ahead of his visit, Gopal contacted the Alumni Relations team at UCL and asked if we could help him find out more about his father's time at the university. We delved into our Special Collections and Student Records to dig out Krishnan's personal files.

Born in 1910, Krishnan studied at UCL during the 1930s. Sadly, Krishnan passed away in 1991 but left a rich legacy for his son to discover. Gopal says: "I remember my father as a kind man, he would always treat people with respect. He was totally dedicated to his profession. He was a spirited man who would not just sit idle. It's always been a mission in my life to see where he studied."

After completing a degree in India, Krishnan studied a Science BSc at UCL from 1931 to 1934 taking on subjects in chemistry and mathematics. Under the direction of His Highness the Maharajah of Travancore (now Kerala), he went on to specialise in rubber technology, becoming an Associate of Rubber Industry, London. He returned to India and was appointed as Rubber Expert in the Travancore Government Rubber Factory, later becoming General Manager before retiring.

While Gopal was visiting, UCL's Special Collections team showed him Krishnan's records, along with some other images and documents from the time he was studying, including the student magazine and photos of the campus. But there was one very special document, Krishnan's student records containing his handwriting and signature. For Gopal, seeing his father's signature after all this time was an incredibly moving moment – and later back in India, Gopal's sisters shed a tear on seeing the photos of it that Gopal had taken.



To give Gopal more perspective on his father's time at UCL, we also took him and Latika behind the scenes of the Chemistry Department, where he met with Professor Andrea Sella and Dr Dewi Lewis.

Gopal and Latika were given a tour of the Chemistry research facilities at the Christopher Ingold Building before being shown the refurbished facilities at the Kathleen Lonsdale Building where

his father would have studied. Gopal shared many photos belonging to his father that showed that not much had changed.

For Gopal, the trip was invaluable. He says: "Those few hours were some of the most memorable moments of my life! I want to express my sincere thanks for all of the wonderful arrangements UCL made, for retaining those records and giving me a chance to see them."

Event photography with thanks from John Moloney Photography Historic images with thanks from Gopal Krishnan. Text from UCL Alumni Relations



Dewi Lewi, Andrea Sella, Gopal and Latika

Photos from last year's Lab dinner



1940 Chemistry Alumni, Leonard Lovelock



After Dinner Speaker Dr Rob Jackson, University of Keele



Prof. Helen Fielding, delivering the 2018 RSC Thomas Graham Lecture

The Kathleen Lonsdale **Schools Lecture**

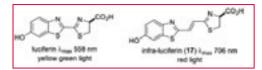
This year we celebrate the 70th anniversary of the appointment of UCL's first female Professor, Dame Kathleen Lonsdale FRS, who was made Professor of Chemistry in 1949. Prof Lonsdale was an eminent crystallographer and social campaigner. discovered the structures of many important molecules and materials, including the first proof that benzene is a planar molecule. With support from the Royal Society of Chemistry, in June we held the first Kathleen Lonsdale Schools Lecture, which was delivered by Prof Judith Howard FRS. This will be an annual event hosted each summer and aimed at encouraging school children into science. We had over 150 students from many local and not-so-local schools attend.

This year's lecture was titled *The Endless Fascination* of Crystals- Kathleen Lonsdale's legacy and Prof Howard gave a great account of Kathleen Lonsdale's life and works. We were also lucky enough to have a talk from Dr. Claire Murray, who is a crystallographer at Diamond Light Source, and also works on the representation of women scientists in school textbooks. Dame Kathleen's son and grandson were also able to attend, as was her last PhD student, Prof. Mike Glazer.

As a department we are glad to have our own 'named lecture' seeing as Imperial and Kings have long established lectures named after their famous alumni. Keep your eyes peeled for the announcement of the 2020 Kathleen Lonsdale Lecture.

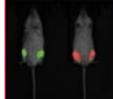
Anderson research lab dual bioluminescence imaging using infraluciferin

The yellow-green light given by firefly's and other insects, known as bioluminescence, is one of nature's most spectacular phenomenon. The light is generated from the combination of a small molecule luciferin with an enzyme, luciferase. The light is spectacularly bright and is regularly used for the imaging of disease in living systems, so that we can see what is going on in real time, without invasion of the system being observed. The gene required to make the enzyme can be introduced into the genome of cells, such as cancer cells. When the cancer grows, the attached DNA machinery of the cell will make the luciferase enzyme. In the presence of luciferin, bioluminescence occurs and the detectable glow shows the extent and progression of the cancer cells. Unfortunately the yellow-green light naturally emitted by fireflys is absorbed by blood and tissue. We synthesised a modified luciferin, infraluciferin, that emits red light, which is transmitted through blood and tissue. Infraluciferin can also emit different shades of red light with modified enzymes. The multicolour red light emission of infraluciferin opens the possibility that we can track multiple biological events in the same sample if they produced different bioluminescence enzymes that emitted different shades of red light. We could then follow different diseases in a living animal or the elimination of a disease by a therapy. This will allow the easier observation of these events which will help develop better cures for diseases, such as cancer, and importantly reduce the number of animals required for the necessary research.



We have been able to show two cancer tumours in a single

mouse, by infraluciferin emitting two different wavelengths of red light. The image below shows two cancer models differentiated by different bioluminescence light emissions with infraluciferin from different enzymes FLuc_green ~700nm (left mouse) and FLuc_red ~720nm (right mouse).



We have also used infraluciferin to track the effectiveness of CAR T cell therapy to eliminate a lymphoma tumour in a living mouse.

Infraluciferin will be used by scientists to study disease in living animals more quickly, cheaply and efficiently. The study of these diseases will enable therapies to be developed to combat them. The effectiveness of the therapies could also be tracked by this technique to help in the faster development of cures.

The Plastic Waste Innovation Hub

The Plastic Waste Innovation Hub was recently launched as a cross-disciplinary project across a number of UCL departments, including the Department of Chemistry (https://www.instituteofmaking.org.uk/blog/2019/04/launch-of-ucl-plastic-waste-innovation-hub).

The Hub was set up as part of a 'Designing-out Plastic Waste' project funded by the Engineering and Physical Sciences Research Council (EPSRC) and UK Research and Innovation (UKRI) to investigate new interventions to tackle plastic waste (https://www. plasticwastehub.org.uk/). Research within the Department in the Hailes group focuses on the use of newly discovered PETases to break down polyethylene terephthalate (PET), whilst simultaneously exploring the use of enzymes for the breakdown of other plastics such as polypropylene and polyethylene. Building on previous work [e.g. F. Subrizi et al, Angew. Chem. Int. Ed., 2019, 58, 3854] upgrading of plastic monomers and the synthesis of novel monomers using enzymes is also ongoing. As part of the project, the team recently gave a talk at Cheltenham Science Festival, discussing possible solutions to the plastic waste problem and presenting our approach to the wider public. The talk aimed to engage the audience in a discussion about the sheer volume of plastic waste we are sending to landfill in the UK and what this means for the future, whilst going on to discuss the possibility of going 'plastic-free' together with misinformation about compostable and biodegradable packaging. Whilst acknowledging that there are many areas in our lives where we can significantly cut down on unnecessary single use plastic, it is important to realise that plastics usage can still be the most efficient option available to us due to its





Caption: From left to right: Charnett Chau, Leona Leipold, Zoe Laughlin and Mark Miodownik

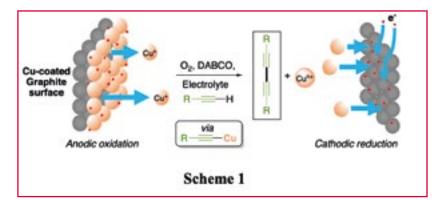
low mass. This is important when considering the wider effects of for example goods transport on climate change and global warming. Equally, the use of compostable and biodegradable plastics is largely misleading, as most countries do not have the industrial composters required for their degradation and they are contaminating current recycling streams or accumulating in the environment. Therefore, we believe that one of the options is to move away from the current linear economy and close the loop by breaking down plastics to their initial monomers to feed back into the system to create recycled virgin plastics.

Applying electricity to classic organic reactions for a green and sustainable future

Jon Wilden

Electricity is a natural force that mankind has successfully harnessed to tremendous benefit. Until recently however, this powerful source of energy has received little attention from organic chemists as a way of controlling their reactions. There are many reasons for this: The apparatus is perceived as being cumbersome and expensive and many see the electrochemical technique as complex and loaded with unfamiliar jargon. The advantages of applying electricity to organic reactions however are considerable. Specific addition or removal of an electron from a substrate can give rise to reactive species that are not accessible by conventional routes. In addition, the sequential nature of the electron transfer reactions offers opportunities for control of reactivity of species participating in reactions.

In 2016, Jon Wilden's group took the decision to refocus their research and focus their efforts on using electricity to effect organic reactions in a 'green' and sustainable way. Initially, copper(I) acetylides were prepared electrochemically which were then subsequently employed in organic C–C bond forming reactions. The group has also demonstrated that application of Faraday's laws allows the charge to be calculated so that only the required amount of metal is used. In addition, the application of copper-coated graphite electrodes allows the maximum atom efficiency for this process and even offers a recovery strategy to extract the metal following completion of the reaction (**Scheme 1**, see Seavill, P. W.; Holt, K. B.; Wilden, J. D. *Green Chem.* **2018**, *20*, 5474-5478).



Recent work within the group has focused on the activation of molecular oxygen via single-electron reduction at a carbon electrode to generate reactive oxygen species capable of selectively activating organic molecules at specific sites in their structure. A key consideration of this approach are the use of benign and non-toxic reagents and additives that are sustainable both environmentally and in terms of energy efficiency. This is particularly important as the functionalisation and manipulation of organic molecules is a critical part of many industries, most notably

pharmaceuticals, agrochemicals and polymer industries. These enterprises are constantly seeking new, sustainable, economical and non-toxic processes to effect construction of organic frameworks. This work has recently secured a grant from the Leverhulme Trust for the group to continue its exploration of this exciting area.

Dr Bob Schroeder awarded UKRI Future Leaders Fellowships

The UK Government have announced funding for 78 scientists and researchers through their Future Leaders Fellowships scheme.

The Government announced a £98 million investment, allowing both UK researchers and small businesses to seize the vast opportunities in science and innovation and industries of the future. Of this,

£78 million will be invested in 78 scientists and researchers, supporting many of those working at the cutting edge of the next scientific discoveries – including solutions to climate change and birth defects.

Dr Schroeder's project will drive advances in self-healing materials, creating a wearable sensor that can be directly applied to human skin to allow for continuous patient monitoring and ultimately improve treatments.

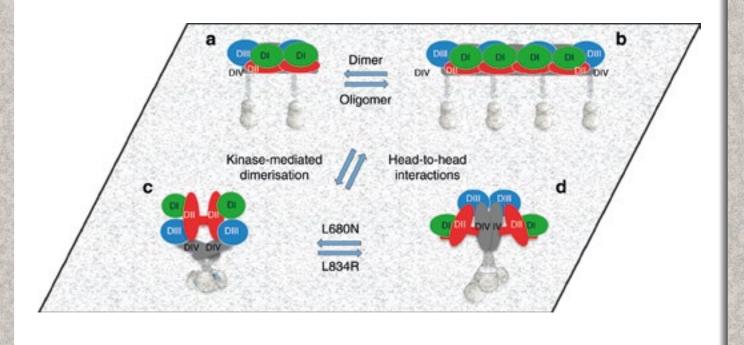
Understanding the activation mechanisms of a crucial drug target for lung cancer

Prof. Francesco L. Gervasio

The simulations performed by Prof. Francesco L. Gervasio's group contributed to clarify the complex activation and autoinhibition mechanisms of Epidermal Growth Factor Receptor through dimers and oligomers.

Epidermal growth factor receptor (EGFR) is a receptor tyrosine kinase whose activation through genetic mutations has been associated with a range of diseases, most notably non-small cell lung cancer. The majority of information regarding EGFR's activation mechanism thus far came from X-ray structures of monomer and dimer receptor fragments which were insufficient to adequately explain the receptor's (mis)behaviour in cells. So far it was thought that the activation of EGFR proceeded through the formation of an asymmetric dimer. Through a variety of high-resolution imaging techniques performed by Dr. Marisa Martin-Fernandez (Oxford and Harwell) combined with the state-of-theart simulation and modelling approaches provided by Prof. Gervasio's group, it was possible to shed light on a much more complex mechanism, where an intricate balance exists between a multitude of EGFR's ligand-free dimeric and even oligomeric forms. This balance is disrupted when the somatic mutations occur in the absence of ligands and the scales are tipped towards active dysregulated forms leading to cell proliferation. These findings, published recently in **Nature Communications**, have great implications in the anti-cancer drug discovery process as they provide novel outlooks on the EGFR's activation in cells and might lead to the design of novel drugs.

Zanetti-Domingues LC, et al. (2018). The architecture of EGFR's basal complexes reveals autoinhibition mechanisms in dimers and oligomers. **Nat Commun** 9, 4325.



Peptide synthesis at the origins of life: energy-rich aminonitriles by-pass deactivated amino acids completely

Saidul Islam & Matthew Powner

Peptides are an essential element of all life on Earth. They are so highly enmeshed in physiology that it is difficult to imagine life without them. Peptide biosynthesis is now orchestrated by a complex host of genetically encoded enzymes, but it is inconceivable that these sophisticated and coordinated macromolecules suddenly emerged at the origin of life. A simpler scenario must lie at the root of peptide biosynthesis, but can the innate reactivity of prebiotic molecules initially replace enzymes? Can chemical reactivity control selective peptide ligation in water?

Peptides are widely assumed to be products of amino acid polymerization reactions. Whilst conceptually simple, in practice there are good reasons why these reactions are ineffective in water. For example, amino acids (pK_{aH} = 9.4) are zwitterionic at physiological pH, which quenches their nucleophilicity by protonation, and electrophilic condensation agents that activate amino acid monomers can irrevocably block peptide synthesis as well as derivatise amino acid side chain residues.

As reported in Nature, our group has reported a method to overcome several long-standing problems of peptide synthesis in water, which avoids uncontrolled polymerization reactions and by-passes amino acids altogether [1].

We took our initial cues from biology. Whereas chemical peptide syntheses generally proceed from the C-to-N terminus with ligation occurring at the activated monomer, both ribosomal (RNA-mediated) and non-ribosomal (thioester-mediated) peptide biosynthesis proceeds from the N-to-C terminus with ligation occurring at the activated C-terminus of the peptide chain (Fig. 1).

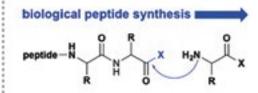


Figure 1 | Peptide synthesis. Chemical peptide synthesis generally proceeds from the C-to-N terminus and requires a two-stage protecting-group strategy with orthogonal protecting groups for the activated monomers alpha-

amine (orange) and the amino acid residues (red). Conversely, biological peptide synthesis proceeds from the N-to-C terminus without protecting groups. PG = protecting group, R = amino acid side chain, X = leaving group.

As life has twice alighted on the same solution, it suggested to us that N-to-C-ligation may be privileged, and we suspected it would also be key to achieving prebiotic peptide synthesis in water. Furthermore, prokaryotic and mitochondrial protein syntheses are both initiated by N-formylation, and over 80% of eukaryote proteins are N-acetylated. Peptide N-acylation appears essential to prevent DKP-induced peptide degradation, so it seemed to us that peptide synthesis should proceed from the *N*-to-*C* terminus and be initiated by *N*-acylation.

But what substrates should be ligated and how should the peptide C-terminus be activated? We suspected that aminonitriles were the missing piece of this puzzle.

Aminonitriles have been widely explored as precursors of amino acids [2][3], but their potential in peptide ligation has been largely overlooked. alpha-Aminonitriles have a remarkably low basicity (pK_{aH} = 5.3) and they are only protonated in acidic solution (Fig. 2), which makes them ideally suited to ligation at physiological pH.

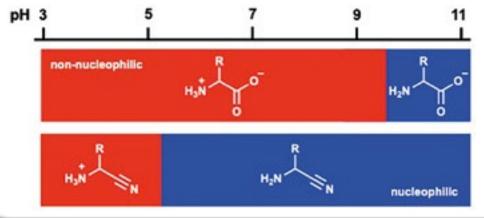


Figure 2 | Nucleophilicity in water. Amino acids are zwitterionic and their nucleophilicity is quenched by protonation at near neutral pH (red), whereas alpha-aminonitriles are only protonated in acidic solution. alpha-Aminonitriles are nucleophilic over abroad pH range (blue), making them ideally suited to peptide ligation at neutral pH.

Additionally, aminonitriles have built-in energy (in their triple bond) that can be harnessed during peptide synthesis, unlike amino acids, which are their deactivated hydrolysis products. Drawing on our previous experience using thioacid activation to direct chemoselective 3'-5'-RNA ligation [4] and nitriles in prebiotic nucleotide synthesis [5][6], as well as recognising the potential commonality between peptide and nucleic acid chemistry, we began to investigate the irresistible opportunity that thioacid chemistry could also ligate alpha-aminonitriles to yield peptides in water.

Upon considering thioacids for peptide synthesis, we were immediately struck by the orthogonal reactivity of phosphates and sulfides, and the opportunities that sulfides opened for selective peptide ligation in a chemical network that needs to simultaneously build peptides and nucleic acids. Lipmann [7] and de Duve [8] had both previously proposed thioester-dependent peptide synthesis preceded RNA-dependent protein synthesis during the evolution of life. This "thioester world hypothesis" is a popular theory in origins of life research, but there had been very little progress in finding a robust prebiotic mechanism to synthesise the thioesters that are required to underpin this whole concept. We suspected this may have been due to a misplaced focus on amino acids and thioesters, rather than on aminonitriles and thioacids.

We found that thioacetate not only quantitatively acetylated alpha-aminonitriles in water, but that acylation electronically activated the nitrile group of the newly formed alpha-amidonitrile just enough to favour nucleophilic attack by H₂S, but not by water. The resulting alpha-amidothioamide was then readily hydrolysed to afford a C-terminal amidothioacid which can be ligated with another alpha-aminonitrile, and so the process can be cycled to yield an iterative peptide ligation in water (Fig. 3) [1].

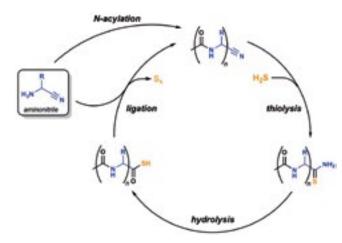


Figure 3 | Peptide ligation cycle. Sulfide-mediated peptide synthesis by N-to-C terminal ligation of aminonitriles in water.

All 20 proteinogenic side chain residues were tolerated (and gave high yields) in amidothioacid ligation, including histidine, aspartate, cysteine, serine, threonine, and tyrosine, which are essential to enzyme catalysis but are notoriously difficult to couple by previously reported (prebiotic) peptide bond forming reactions. The low basicity of alpha-aminonitriles even permits selective ligation of lysine residues to give natural alpha-peptide bonds. This lysine selectivity derives from the ~5 orders of magnitude difference in basicity of the two amine moieties of lysine nitrile. And finally, because our strategy operates via C-terminal peptide activation, rather than monomer activation, peptide fragment ligation is just as

effective as monomer ligation by our strategy, which provides a mechanism to rapidly build larger peptides [1].

Our results provide yet another clue that implicates cyanosulfidic chemistry at the origin of life [1][2][4][5][6][9][10], and we are currently developing other variants of our aminonitrile ligation. We are also exploring the emergence of function in these systems to further validate the prebiotic credentials of our chemistry.

Nevertheless, our results already have broad implications for understanding the origins of life. The highly predisposed nature of these reactions, under simple mild aqueous conditions, suggests that the chemistry of cyanide and sulfide foreshadowed enzyme-controlled peptide biosynthesis pathways.

This research has been published in Nature.

References:

- [1] Canavelli, P., Islam, S. & Powner, M. W. Nature (2019).
- [2] Islam, S., Bucar, D.-K. & Powner, M. W. Nat. Chem. 9, 584-589 (2017).
- [3] Islam, S. & Powner M. W. Chem 2, 470-501 (2017).
- [4] Bowler, F. R. et al. Nat. Chem. 5, 383-389 (2013).
- [5] Powner, M. W., Gerland, B. & Sutherland, J. D. Nature 459, 239-242 (2009).
- [6] Stairs, S. et al. Nat. Commun. 8, 15270 (2017).
- [7] Lipmann, F. Science 173, 875–884 (1971).
- [8] de Duve, C. Blueprint For a Cell: The Nature and Origin of Life (Neil Patterson Publishers, Burlington, NC) (1991).
- [9] Patel, B. H. et al. Nat. Chem. 7, 301-307 (2015).
- [10] Roberts, S. et al. Nat. Commun. 9, 4073 (2018).

Grants and Awards

Studies of radical-surface chemistry of relevance to the interstellar medium

£177961.00 Leverhulme Trust

PI: Professor Stephen Price

1 October 2018

Understanding how the microenvironment of a protein can dictate the course of bioconjugation

£154274.00

Leverhulme Trust

PI: Dr Vijay Chudasama

1 August 2018

Probing novel doping mechanisms for high mobility transparent conducting oxides

£44214.00

Diamond Light Source Ltd

PI: Professor David Scanlon

1 October 2018

Neuro-oncological precision nanomedicines

£780882.44 EPSRC

PI: Professor Giuseppe Battaglia

2 September 2018

High end computing materials chemistry consortium

£489,315.64

EPSRC
PI: Professor Scott Woodley

1 November 2019

A combined activation/tethering strategy to lariat peptides

£185,286

Leverhulme Trust

PI: Dr Derek Macmillan

3 September 2018

Developing inkjet printable electronics inks and coatings

£100,000 EPSRC

PI: Professor Jawwad Darr

1 October 2018

Understanding structure evolution in supported metal nanoparticles used in emission control; translating observations made on model catalysts to real world applications

£20,000

Diamond Light Source Ltd

PI: Professor Andrew Beale

1 October 2019

Understanding Structure Evolution in Supported metal nanoparticles used in emission control; translating observations made on model catalysts to real world applications

£16,000

Johnson Matthey

PI: Professor Andrew Beale

1 October 2018

Depollution of air using polymer-based coatings

£213,033 Innovate UK

PI: Professor Andrew Beale

1 September 2019

Sustainable Manufacturing of Transparent Conducting Oxide (TCO) Thin Films

£99,784 EPSRC

PI: Professor Claire Carmalt

1 September 2018

Multiphoton UV photoelectron spectroscopy in liquid microjets

£52650.42 Royal Society

PI: Professor Helen Fielding

1 October 2018

Coordinated Swarm Behaviour with Minimal Communication in Complex Topographies

£54,080.77

Office of Naval Research

PI: Dr Giorgio Volpe

1 October 2018

Prebiotic synthesis on the rocks

£311,440

Volkswagen Stiftung

PI: Dr Matthew Powner

1 September 2018

Cold press sintering of Solid State Electrolyte powders

£50,000 EPSRC

PI: Professor Jawwad Darr

1 November 2018

Ionic Liquid Lubricants

£34,000 Edwards Ltd

PI: Dr Robert Palgrave

1 October 2018

The PowerPI: Drive Line

£746,211.05 Innovate UK

PI: Professor Jawwad Darr

1 October 2018

Designed Synthesis of Zeolites for Environmental and Biorenewables Catalysis

£318.462 **EPSRC**

PI: Professor Andrew Beale

1 December 2018

Development of a polymersome treatment for brain cancer

£96.204

EPSRC - IMPACT ACCELERATION ACCOUNT

PI: Professor Giuseppe Battaglia

1 November 2018

The Development of In Situ Soft XAS Capabilities in the UK; exemplification Via Understanding The **Dynamic Nature Of Fischer-Tropsch Synthesis** Catalysts (Diamond)

£40.000

Johnson Matthey

PI: Professor Andrew Beale

1 November 2018

The development of in situ soft XAS capabilities in the UK; exemplification via understanding the dynamic nature of Fischer-Tropsch synthesis catalysts (JM)

£25,000 Diamond

PI: Professor Andrew Beale

1 November 2018

Easy-to-clean Antimicrobial Superhydrophobic Coatings

£36.000

Altro Limited

PI: Professor Claire Carmalt

24 September 2018

Determining the mechanism of piston deposit formation

£45,000

Infineum International Ltd

PI: Professor Andrew Beale

1 October 2018

Polymersomes for cancer immune-therapy applications

£70,000

BTG International Ltd

PI: Professor Giuseppe Battaglia

1 October 2018

Protometabolic pathways: exploring the chemical roots of systems biology

£225.258.05

European Commission H2020-H2020-MSCA-ITN-2018

PI: Dr Matthew Powner

1 November 2018

Designing-out Plastic Waste

£171,353.59 **EPSRC**

PI: Professor Helen Hailes

1 January 2019

Concerted action for the European HPC CoEs

£217,200

European Commission

PI: Professor Peter Coveney

1 December 2018

Towards Safer Hospitals: Bioaerosol surveillance system

£29,996

EPSRC - Impact Acceleration Account

PI: Dr Daren Caruana

7 May 2019

Workshop: Complex Nanophotonics at the Interface

£10,822 **EPSRC**

PI: Dr Giorgio Volpe

15 July 2019

Accelerating Tau PET Imaging through Head to Head Comparison of Novel Radiotracers

£99,042.90

Fidelity Biosciences

PI: Dr Kerstin Sander

1 March 2019

Accelerating Tau PET Imaging through Head to **Head Comparison of Novel Radiotracers**

Association for Frontotemporal Degeneration (AFTD)

PI: Dr Kerstin Sander

1 March 2019

Synthetic Peptidic Nanovesicles for Targeting **Paediatric Brain tumours**

£146.763.84

European Commission H2020-MSCA-IF-2017

PI: Professor Giuseppe Battaglia

1 April 2019

Nanopores DNA Origami Single Molecule Protein Analysis Biotechnology

£22.000

Oxford Nanopore Technologies Ltd

PI: Professor Stefan Howorka

24 September 2018

Supramolecular conjugated polymers - a new approach towards electronic skin

£20,000

Royal Society

PI: Dr Bob Schroeder

27 March 2019

GRANTS AND AWARDS

Development of Raman spectroscopy technologies for in vivo and ex vivo assessment of tissue samples.

£29,112.16 **MRC**

PI: Professor Paul McMillan

1 April 2019

Rational design of photoactive molecules using "black box" quantum dynamics simulations £392,509.0

EPSRC

PI: Professor Graham Worth

1 May 2019

Systems Chemistry: Unified Metabolite Syntheses at the Origin of Life

£109.7175.86 Simons Foundation PI: Dr Matthew Powner

1 June 2019

Global warming amelioration by oxidation of methane

£10,000

UK British Council

PI: Professor Chris Blackman

1 April 2019

The department ran a summer 'Photography as art competition' for all PHD and post docs. There were two categories: In the Lab and Chemistry Up Close.

The winners of £25 Amazon vouchers were:

Viliyana Tsanova with her photo titled: Frankie says

relax' a photo taken of the labs relaxometer from above.



Clara Sanchez-Perez with her photo of a new single-

source precursor developed in the Carmalt group for the deposition of novel bismuthbased perovskite materials for solar cells with improved stability.



Abe R, Aitchison CM, Andrei V, Beller M, Cheung D, Creissen CE, de la Peña O'Shea VA, Durrant JR, Grätzel M, Hammarström L, Haussener S, In S-I, Kalamaras E, Kudo A, Kuehnel MF, Kunturu PP, Lai Y-H, Lee C-Y, Maneiro M, Moore EE, Nguyen HC, Paris AR, Pornrungroj C, Reek JNH, Reisner E, Schreck M, Smith WA, Soo HS, Sprick RS, Venugopal A, Wang Q, Wielend D, **Zwijnenburg MA**, Demonstrator devices for artificial photosynthesis: general discussion, *Faraday Discussions*, 2019, **215**, 345-363

Addicoat M, Adjiman CS, Arhangelskis M, Beran GJO, Bowskill D, Brandenburg JG, Braun DE, Burger V, Cole J, Cruz-Cabeza AJ, Day GM, Deringer VL, Guo R, Hare A, Helfferich J, Hoja J, Iuzzolino L, Jobbins S, Marom N, McKay D, Mitchell JBO, Mohamed S, Neumann M, Nilsson Lill S, Nyman J, Oganov AR, Piaggi P, Price SL, Reutzel-Edens S, Rietveld I, Ruggiero M, Ryder MR, Sastre G, Schön JC, Taylor C, Tkatchenko A, Tsuzuki S, van den Ende J, Woodley SM, Woollam G, Zhu Q, Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion, Faraday Discussions, 2018, **211**, 325-381

Addicoat M, Adjiman CS, Arhangelskis M, Beran GJO, Brandenburg JG, Braun DE, Burger V, Burow A, Collins C, Cooper A, Day GM, Deringer VL, Dyer MS, Hare A, Jelfs KE, Keupp J, Konstantinopoulos S, Li Y, Ma Y, Marom N, McKay D, Mellot-Draznieks C, Mohamed S, Neumann M, Lill SN, Nyman J, Oganov AR, Price SL, Reutzel-Edens S, Ruggiero M, Sastre G, Schmid R, Schmidt J, Schon JC, Spackman P, Tsuzuki S, Woodley SM, Yang S, Zhu Q, Structure searching methods: general discussion, *Faraday Discussions*, 2018, 211, 133-180

Adishev A, Arrigo R, Baletto F, Bordet A, Bukhtiyarov V, Carosso M, **Catlow R**, Conway M, Davies J, Davies P, De Masi D, Demirci C, Edwards JK, Friend C, Gallarati S, Hargreaves J, Huang H, Hutchings G, Lai S, Lamberti C, Macino M, Marchant D, Murayama T, Odarchenko Y, Peron J, Prati L, Quinson J, Richards N, Rogers S, Russell A, Selvam P, Shah P, Shozi M, Skylaris C-K, Soulantica K, Spolaore F, Tooze B, Torrente-Murciano L, Trunschke A, Venezia B, Walker J, Whiston K, Control of catalytic nanoparticle synthesis: general discussion, *Faraday Discussions*, 2018, **208**, 471-495

Adjiman CS, Brandenburg JG, Braun DE, Cole J, Collins C, Cooper AI, Cruz-Cabeza AJ, Day GM, Dudek M, Hare A, Iuzzolino L, McKay D, Mitchell JBO, Mohamed S, Neelamraju S, Neumann M, Nilsson Lill S, Nyman J, Oganov AR, **Price SL**, Pulido A, Reutzel-Edens S, Rietveld I, Ruggiero MT,

Schön JC, Tsuzuki S, van den Ende J, Woollam G, Zhu Q, Applications of crystal structure prediction - organic molecular structures: general discussion, *Faraday Discussions*, 2018, **211**, 493-539

Adjogatse E, Erskine P, Wells SA, Kelly JM, Wilden JD, Chan AWE, Selwood D, Coker A, Wood S, Cooper JB, Structure and function of L-threonine-3-dehydrogenase from the parasitic protozoan Trypanosoma brucei revealed by X-ray crystallography and geometric simulations, *Acta Crystallographica Section D*, 2018, **74**, 861-876

Agote-Arán M, Kroner AB, Islam HU, Sławiński WA, Wragg DS, Lezcano-González I, **Beale AM**, Determination of Molybdenum Species Evolution during Non-Oxidative Dehydroaromatization of Methane and its Implications for Catalytic Performance, *ChemCatChem*, 2018, **11**, 473-480

Agote-Arán M, Lezcano-González I, Greenaway AG, Hayama S, Díaz-Moreno S, Kroner AB, **Beale AM**, Operando HERFD-XANES/XES studies reveal differences in the activity of Fe-species in MFI and CHA structures for the standard selective catalytic reduction of NO with NH3, *Applied Catalysis A: General*, 2019, **570**, 283-291

Aina AA, Misquitta AJ, Phipps MJS, **Price SL**, Charge Distributions of Nitro Groups Within Organic Explosive Crystals: Effects on Sensitivity and Modeling, *ACS Omega*, 2019, **4**, 8614-8625

Aitchison CM, Andrei V, Antón-García D, Apfel U-P, Badiani V, Beller M, Bocarsly AB, Bonnet S, Brueggeller P, Caputo CA, Cassiola F, Clausing ST, Cooper AI, Creissen CE, de la Peña O'Shea VA, Domcke W, Durrant JR, Grätzel M, Hammarström L, Hankin A, Hatzell MC, Karadas F, König B, Kuehnel MF, Lamaison S, Lin C-Y, Maneiro M, Minteer SD, R Paris A, Pastor E, Pornrungroj C, Reek JNH, Reisner E, Roy S, Sahm C, Shankar R, Shaw WJ, Shylin SI, Smith WA, Sokol K, Soo HS, Sprick RS, Viertl W, Vogel A, Wagner A, Wakerley D, Wang Q, Wielend D, Zwijnenburg MA, Synthetic approaches to artificial photosynthesis: general discussion, Faraday Discussions, 2019, **215**, 242-281

Aliev AE, **Motherwell WB**, Some Recent Advances in the Design and Use of Molecular Balances for the Experimental Quantification of Intramolecular Noncovalent Interactions of π Systems, *Chemistry*, 2019, **25**, 10516-10560

Alowayyed S, Piontek T, Suter JL, Hoenen O, Groen D, Luk O, Bosak B, Kopta P, Kurowski K, Perks O, Brabazon K, Jancauskas V, Coster D, **Coveney PV**, Hoekstra AG, Patterns for High Performance Multiscale Computing, Future Generation Computer Systems, 2019, **91**, 335-346

Alqahtani M, Ben-Jabar S, Ebaid M, Sathasivam S, Jurczak P, Xia X, Alromaeh A, Blackman CS, Qin Y, Zhang B, Ooi BS, Liu H, **Parkin IP**, Wu J, Gallium Phosphide photoanode coated with TiO₂ and CoO_x for stable photoelectrochemical water oxidation, *Optics Express*, 2019, **27**, A364-A371

Alqahtani M, Sathasivam S, Alhassan A, Cui F, Benjaber S, **Blackman C**, Zhang B, Qin Y, Parkin IP, Nakamura S, Liu H, Wu J, InGaN/GaN Multiple Quantum Well Photoanode Modified with Cobalt Oxide for Water Oxidation, *ACS Applied Energy Materials*, 2018, **1**, 6417-6424

Alqahtani M, Sathasivam S, Cui F, Steier L, Xia X, **Blackman C**, Kim E, Shin H, Benamara M, Mazur YI, Salamo GJ, Parkin IP, Liu H, Wu J, Heteroepitaxy of GaP on silicon for efficient and costeffective photoelectrochemical water splitting, *Journal of Materials Chemistry A*, 2019, **7**, 8550-8558

Ambroz F, Macdonald TJ, Martis V, **Parkin IP**, Evaluation of the BET Theory for the Characterization of Meso and Microporous MOFs, *Small Methods*, 2018, **2**, 1800173

Ambroz F, Sathasivam S, Lee R, Gadipelli S, Lin CT, Xu S, Poduval RK, Mclachlan MA, Papakonstantinou I, **Parkin IP**, Macdonald TJ, Influence of Lithium and Lanthanum Treatment on TiO₂ Nanofibers and Their Application in n-i-p Solar Cells, *ChemElectroChem*, 2019, **6**, 3590-3598

Andac T, Weigmann P, Velu SKP, Pinçe E, Volpe G, **Volpe G**, Callegari A, Active matter alters the growth dynamics of coffee rings, *Soft Matter*, 2019, **15**, 1488-1496

Anderson JC, Chang C-H, Jathoul AP, Syed AJ, Synthesis and bioluminescence of electronically modified and rotationally restricted colour-shifting infraluciferin analogues, *Tetrahedron*, 2019, **75**, 347-356

Anderson SL, Boyd PG, Gladysiak A, Nguyen TN, **Palgrave RG**, Kubicki D, Emsley L, Bradshaw D, Rosseinsky MJ, Smit B, Stylianou KC, Nucleobase pairing and photodimerization in a biologically derived metal-organic framework nanoreactor, *Nature Communications*, 2019, **10**, 1612

PUBLICATIONS

Aniagyei A, Dzade NY, Tia R, Adei E, Catlow CRA, De Leeuw NH, Ab initio investigation of O₂ adsorption on Cadoped LaMnO3 cathodes in solid oxide fuel cells, Physical Chemistry Chemical Physics, 2018, 20, 28685-28698

Armer CF, Lübke M, Johnson I, McColl K, Cora F, Yeoh JS, Reddy MV, Darr JA, Li X, Lowe A, Enhanced electrochemical performance of electrospun V2O5 fibres doped with redox-inactive metals. Journal of Solid State Electrochemistry, 2018, 22, 3703-3716

Arnott PM, Howorka S, A Temperature-Gated Nanovalve Self-Assembled from **DNA to Control Molecular Transport** across Membranes, ACS Nano, 2019, 13, 3334-3340

Arnott PM, Joshi H, Aksimentiev A, Howorka S, Dynamic Interactions between Lipid-Tethered DNA and Phospholipid Membranes, Langmuir, 2018, 34, 15084-15092

Arrigo R, Badmus K, Baletto F, Boeije M, Bowker M, Brinkert K, Bugaev A, Bukhtiyarov V, Carosso M, Catlow R, Chanerika R, Davies PR, Dononelli W, Freund H-J, Friend C, Gallarati S, Gates B, Genest A, Gibson EK, Hargreaves J, Helveg S, Huang H, Hutchings G, Irvine N, Johnston R, Lai S, Lamberti C, Macginley J, Marchant D, Murayama T, Nome R, Odarchenko Y, Quinson J, Rogers S, Russell A, Said S, Sermon P, Shah P, Simoncelli S, Soulantica K, Spolaore F, Tooze B, Torrente-Murciano L, Trunschke A, Willock D, Zhang J, The challenges of characterising nanoparticulate catalysts: general discussion, Faraday Discussions, 2018, 208, 339-394

Arrigo R, Badmus K, Baletto F, Boeije M, Brinkert K, Bugaev A, Bukhtiyarov V, Carosso M, Catlow R, Chutia A, Davies P, de Leeuw N, Dononelli W, Freund H-J, Friend C, Gates B, Genest A, Hargreaves J, Hutchings G, Johnston R, Lamberti C, Marbaix J, Miranda CR, Odarchenko Y, Richards N, Russell A, Selvam P, Sermon P, Shah P, Shevlin S, Shozi M, Skylaris C-K, Soulantica K, Torrente-Murciano L, Trunschke A, van Santen R, Verga LG, Whiston K, Willock D, Theory as a driving force to understand reactions on nanoparticles: general discussion, Faraday Discussions, 2018, 208, 147-185

Askin S, Cockcroft J, Price SL, Goncalves A, Zhao M, Tocher D, Williams G, Gaisford S, Craig D, Olanzapine form IV: discovery of a new polymorphic form enabled by computed crystal energy landscapes, Crystal Growth and Design, 2019, 19, 2751-2757

Attanzio A, Rosillo-Lopez M, Zampetti A, lerides I, Cacialli F, Salzmann CG, Palma M, Assembly of graphene nanoflake-quantum dot hybrids in aqueous solution and their performance in light-harvesting applications, Nanoscale, 2018, 10, 19678-19683

Hart E, Jodray M, Rodriguez K, Barrera M, Qian E, Zha O, Tong X Y, Woods D. Liu Y, Lee G, Acree W E Jr, and Abraham MH, Model correlations for describing the solubilizing character of 3-methoxy-1-butanol and 1-tert-butoxy-2propanol solvents, Phys. Chem. Liquids, 2019, **57**, 163-173

Babikov D, Benoit D, Bowman J, Burd T, Clary D, Donovan R, Fischer I, Gianturco F, Hochlaf M, Kar S, Kirrander A, Leone S, Malcomson T, Manthe U, McCoy AB, Petersen J, Richardson J, Slavíček P, Stoecklin T, Szalewicz K, van der Avoird A, Wester R, Worth G, Zehnacker-Rentien A, Quantum dynamics of isolated molecules: general discussion, Faraday Discussions, 2018, 212, 281-306

Bacic Z, Benoit D, Besemer M, Bowman J, Bradforth S, Clary D, Donovan R, Fischer I, Gianturco F, Hochlaf M, Houston P, Knowles P, Leone S, Linguerri R, Manthe U, McCoy AB, Petersen J, Richardson J, Shan X, Slavíček P, Stoecklin T, Szalewicz K, van der Avoird A, Wester R, Worth G, Zehnacker-Rentien A, Precise characterisation of isolated molecules: general discussion, Faraday Discuss, 2018, 212, 137-155

Badiani V, Bajada M, Beller M, Bocarsly AB, Bonnet S, Bozal-Ginesta C, Brueggeller P. Butt JN, Cassiola F. Grätzel M, Hammarström L, Hatzell MC, Jeuken LJC, König B, Kuehnel MF, Lawrence J, Lee C-Y, Maneiro M, Minteer SD, Moore EE, Piper SEH, Plumeré N, Reek JNH, Reisner E, Roy S, Shears J, Shylin SI, Soo HS, Wagner A, Wielend D, Zhang J, Zwijnenburg M, Biological approaches to artificial photosynthesis: general discussion, Faraday Discussions, 2019, 215, 66-83

Baharudin KB, Taufiq-Yap YH, Hunns J, Isaacs M, Wilson K, Derawi D, Mesoporous NiO/Al-SBA-15 catalysts for solvent-free deoxygenation of palm fatty acid distillate, Microporous and Mesoporous Materials, 2019, 276, 13-22

Bahmani F, Kazemi SH, Wu Y, Liu L, Xu Y, Lei Y, CuMnO₂-reduced graphene oxide nanocomposite as a freestanding electrode for high-performance supercapacitors, Chemical Engineering Journal, 2019, 375, 121966

Bahou C, Love EA, Leonard S, Spears RJ, Maruani A, Armour K, Baker JR, Chudasama V, Disulfide Modified IgG1: An Investigation of Biophysical Profile and Clinically Relevant Fc Interactions., Bioconjugate Chemistry, 2019, 30, 1048-

Bai Y, Wilbraham L, Slater B, Zwijnenburg MA, Sprick RS, Cooper A, Accelerated discovery of organic polymer photocatalysts for hydrogen evolution from water through the integration of experiment and theory, Journal of the American Chemical Society, 2019, 141, 9063-9071

Bakewell C, White A, Crimmin M, Reversible Alkene Binding and Allylic C-H Activation with an Aluminum(I) Complex, Chemical Science, 2019, 10, 2452-2458

Bara D, Wilson C, Mörtel M, Khusniyarov MM, Ling S, Slater B, Sproules S, Forgan RS, Kinetic Control of Interpenetration in Fe-Biphenyl-4,4'-dicarboxylate Metal-Organic Frameworks by Coordination and Oxidation Modulation, Journal of the American Chemical Society, 2019, 141, 8346-8357

Barnett S, Allan D, Gutmann M, Cockcroft JK, Mai VH, Aliev AE, Saßmannshausen J, Combined high resolution X-ray and DFT Bader analysis to reveal a proposed Ru-H...Si interaction in Cp(IPr)Ru(H), SiH(Ph)Cl, Inorganica Chimica Acta, 2019, 488, 292-298

Bashian NH, Zhou S, Zuba M, Ganose AM, Stiles JW, Ee A, Ashby DS, Scanlon DO, Piper LFJ, Dunn B, Melot BC, Correlated Polyhedral Rotations in the Absence of Polarons during Electrochemical Insertion of Lithium in ReO₃, ACS Energy Letters, 2018, **3**, 2513-2519

Bawn M, Subrizi F, Lye GJ, Sheppard TD, Hailes HC, Ward JM, One-pot, two-step transaminase and transketolase synthesis of L-gluco-heptulose from L-arabinose, Enzyme and Microbial Technology, 2018, 116, 16-22

Bawn M, Subrizi F, Lye GJ, Sheppard TD, Hailes HC, Ward JM, Data on a thermostable enzymatic one-pot reaction for the production of a high-value compound from L-arabinose, Data in Brief, 2018, 19, 1341-1354

Bhati AP, Wan S, Coveney PV, Ensemble-based replica exchange alchemical free energy methods: the effect of protein mutations on inhibitor binding, Journal of Chemical Theory and Computation, 2019, 15, 1265-1277

Birkett M, Savory CN, Rajpalke MK, Linhart WM, Whittles TJ, Gibbon JT, Welch AW, Mitrovic IZ, Zakutayev A, **Scanlon DO**, Veal TD, Band gap temperature-dependence and exciton-like state in copper antimony sulphide, CuSbS₂, *APL Materials*, 2018, **6**, 84904

Blunt MO, Hu Y, Toft CW, Slater AG, Lewis W, Champness NR, Controlling the Two-Dimensional Self-Assembly of Functionalized Porphyrins via Adenine-Thymine Quartet Formation, *Journal of Physical Chemistry C*, 2018, **122**, 26070-26079

Tong X, Woods D, Acree WE Jr and **Abraham MH**, Updated Abraham model correlations for correlating solute transfer into dry butanone and dry cyclohexanone solvents, *Physics Chem.Liquids*, 2018, **56**, 571-583

Bofinger R, Zaw-Thin M, Mitchell NJ, Patrick PS, Stowe C, Gomez-Ramirez A, Hailes HC, Kalber TL, Tabor AB, Development of lipopolyplexes for gene delivery: A comparison of the effects of differing modes of targeting peptide display on the structure and transfection activities of lipopolyplexes, *Journal of Peptide Science*, 2018, 24, e3131

Boldrin D, Fak B, Canevet E, Ollivier J, Walker HC, Manuel P, Khalyavin DD, Wills AS, Vesignieite: An S=1/2 Kagome Antiferromagnet with Dominant Third-Neighbor Exchange, *Physical review letters*, 2018, **121**, 107203

Bucar D-K, Friscic T, Professor William Jones and His Materials Chemistry Group: Innovations and Advances in the Chemistry of Solids, *Crystal Growth and Design*, 2019, **19**, 1479-1487

Buckeridge J, **Scanlon DO**, Electronic band structure and optical properties of boron arsenide, *Physical Review Materials*, 2019, **3**, 051601

Burger V, Claeyssens F, Davies DW, Day GM, Dyer MS, Hare A, Li Y, Mellot-Draznieks C, Mitchell JBO, Mohamed S, Oganov AR, **Price SL**, Ruggiero M, Ryder MR, Sastre G, Schön JC, Spackman P, **Woodley SM**, Zhu Q, Applications of crystal structure prediction - inorganic and network structures: general discussion, *Faraday Discussions*, 2018, **211**, 613-642

Burns JR, **Howorka S**, Structural and Functional Stability of DNA Nanopores in Biological Media, *Nanomaterials*, 2019, **9**, E490

Callegari A, Andac T, Weigmann P, Velu SKP, Pince E, **Volpe G**, Volpe G, Active matter alters the growth dynamics of coffee rings, *Soft Matter*, 2019, **15**, 1488-1496

Callison J, Subramanian ND, Rogers SM, Chutia A, Gianolio D, **Catlow CRA**, Wells PP, Dimitratos N, Directed aqueous-phase reforming of glycerol through tailored platinum nanoparticles, *Applied Catalysis B: Environmental*, 2018, **238**, 618-628

Caruana DJ, Calleja M, Elahi A, Gas Phase Electrochemical Analysis of Amino Acids and their Fragments, Communications Chemistry, 2018, 1, 48

Case DH, Srirambhatla VK, Guo R, Watson RE, Price LS, Polyzois H, Cockcroft JK, Florence AJ, Tocher DA, Price SL, Successful computationally-directed templating of metastable pharmaceutical polymorphs, *Crystal Growth and Design*, 2018, **18**, 5322-5331

Cavaye H, Roberts E, **Salzmann CG**, Senesi R, Fernandez-Alonso F, Molecular Spectroscopy Science Meeting – MSSM2018, *Neutron News*, 2019, **29**, 13-15

Chidchob P, Offenbartl-Stiegert D, McCarthy D, Luo X, Li J, **Howorka S**, Sleiman HF, Spatial presentation of cholesterol units on a DNA cube as a determinant of membrane protein-mimicking functions, *Journal of the American Chemical Society*, 2019, **141**, 1100-1108

Chudasama V, Antibody – Drug conjugates (ADC) – Drug discovery today: Technologies, Drug Discovery Today: Technologies, 2018, **30**, 1-2

Chutia A, Willock DJ, **Catlow CRA**, The electronic properties of Au clusters on CeO₂ (110) surface with and without O-defects, *Faraday Discussions*, 2018, **208**, 123-145

Abraham MH and Acree WE Jr, Solvation descriptors for zwitterionic a-aminoacids; estimation of their watersolvent partition coefficients, solubilities and hydrogen-bond acidity and hydrogen-bond basicity, *ACS Omega*, 2019, **4**, 2883-2892

Qian E, Gupta A, Neal R, Lee G, Che M, Wang L, Yue D, Wang S, Liu K, Zhang A, Acree WE Jr and **Abraham MH**, Abraham model correlations for describing solute transfer into 4-methyl-2-pentanol from both water and the gas phase, *J. Molecular Liquids*, 2019, **278**, 335-341

Clancy AJ, Anthony DB, Shaffer MSP, Reactive coagulation of single-walled carbon nanotubes for tougher composites - Solution processing and assembly, *AIP Conference Proceedings*, 2019, **2055**, 090005

Clancy AJ, Bayazit MK, Hodge SA, Skipper NT, Howard CA, Shaffer MSP, Charged Carbon Nanomaterials: Redox Chemistries of Fullerenes, Carbon Nanotubes, and Graphenes, *Chemical Reviews*, 2018, **118**, 7363-7408

Clancy AJ, Sirisinudomkit P, Anthony DB, Thong AZ, Greenfield JL, Salaken Singh MK, Shaffer MSP, Real-time mechanistic study of carbon nanotube anion functionalisation through open circuit voltammetry, *Chemical Science*, 2019, **10**, 3300-3306

Clancy ARJ, Leese H, Rubio N, Buckley D, Greenfield J, Shaffer M, Depleting Depletion: Maintaining Single-Walled Carbon Nanotube Dispersions after Graft-to Polymer Functionalization, Langmuir, 2018, 34, 15396-15402

Coates G, Ward B, **Bakewell C**, White A, Crimmin M, Reactions of Fluoroalkanes with Mg-Mg Bonds: Scope, sp3C-F / sp2C-F Coupling and Mechanism, *Chemistry - A European Journal*, 2018, **24**, 16282-16286

Cockcroft JK, Rosu-Finsen A, Fitch AN, Williams JH, The temperature dependence of C-H...F-C interactions in benzene:hexafluorobenzene, *CrystEngComm*, 2018, **20**, 6677-6682

Contini C, Pearson R, Wang L, Messager L, Gaitzsch J, Rizzello L, Ruiz-Perez L, **Battaglia G**, Bottom-Up Evolution of Vesicles from Disks to High-Genus Polymersomes, *iScience*, 2018, **7**, 132-144

Coomber CE, Laserna V, Martin LT, Smith PD, **Hailes HC**, **Porter MJ**, **Sheppard TD**, Catalytic direct amidations in tert-butyl acetate using B(OCH₂CF₃)₃, *Organic & Biomolecular Chemistry*, 2019, **17**, 6465-6469

Corby S, Francas L, Selim S, Sachs M, **Blackman C**, Kafizas A, Durrant JR, Water Oxidation and Electron Extraction Kinetics in Nanostructured Tungsten Trioxide Photoanodes, *Journal of the American Chemical Society*, 2018, **140**, 16168-16177

Corpinot MK, **Bučar DK**, A Practical Guide to the Design of Molecular Crystals, *Crystal Growth and Design*, 2019, **19**, 1426-1453

Coveney PV, Suter JL, Richardson RA, Sinclair RC, Vassaux M, The Role of Graphene in Enhancing the Material Properties of Thermosetting Polymers, *Advanced Theory and Simulations*, 2019, **2**, 1800168

PUBLICATIONS

Dakka J, Farkas-Pall K, Turilli M, Wright DW, Coveney PV, Jha S, Concurrent and Adaptive Extreme Scale Binding Free Energy Calculations, Proceedings 2018 IEEE 14th International Conference on e-Science (e-Science), 2018, 189-200

Dakka J, Turilli M, Wright DW, Zasada SJ, Balasubramanian V, Wan S, Coveney PV, Jha S, High-throughput binding affinity calculations at extreme scales, BMC Bioinformatics, 2018, 19, 482

Daniels LM, Ling S, Savvin SN, Pitcher MJ, Dyer MS, Claridge JB, Slater B, Corà F, Alaria J, Rosseinsky MJ, A and B site doping of a phonon-glass perovskite oxide thermoelectric, Journal of Materials Chemistry A, 2018, 6, 15640-15652

Dann EK, Gibson EK, Blackmore RH, Catlow CRA, Collier P, Chutia A, Erden TE, Hardacre C, Kroner A, Nachtegaal M, Raj A, Rogers SM, Taylor SFR, Thompson P, Tierney GF, Zeinalipour-Yazdi CD, Goguet A, Wells PP, Structural selectivity of supported Pd nanoparticles for catalytic NH oxidation resolved using combined operando spectroscopy. Nature Catalysis, 2019, 2, 157-163

Dann EK, Gibson EK, Catlow CRA, Celorrio V, Collier P, Eralp T, Amboage M, Hardacre C, Stere C, Kroner A, Raj A, Rogers S, Goguet A, Wells PP, Combined spatially resolved operando spectroscopy: New insights into kinetic oscillations of CO oxidation on Pd/y-Al₂O₃, Journal of Catalysis, 2019-05, 2019, 373, 201-208

Davies DW, Walsh A, Mudd JJ, McConville CF, Regoutz A, Kahk JM, Payne DJ, Dhanak VR, Hesp D, Pussi K, Lee T-L, Egdell RG, Zhang KHL, Identification of Lone-Pair Surface States on Indium Oxide, Journal of Physical Chemistry C, 2019, 123, 1700-1709

Acree WE Jr, Smart K and Abraham MH, Abraham model solute descriptors reveal strong intramolecular hydrogen bonding in 1,4-dihydroxyanthraquinone and 1,8-dihydroxyanthraquinone, Phys. Chem. Liquids, 2018, 56, 416-420

Davies G.-L., Guldin S, Patel M, Harman C, Recent Developments in Pickering Emulsions for Biomedical Applications, Current Opinion on Colloid and Interface Science, 2019, 39, 173-189

Dimitrov S, Azzouzi M, Wu J, Yao J, Dong Y, Shakya Tuladhar P, Schroeder BC, Bittner E, McCulloch I, Nelson J, Durrant J. Spectroscopic Investigation of the Effect of Microstructure and Energetic Offset on the Nature of Interfacial Charge Transfer States in Polymer: Fullerene Blends, Journal of the American Chemical Society, 2019, 141, 4634-4643

Dong H, Xu Y, Zhang C, Wu Y, Zhou M, Liu L, Dong Y, Fu Q, Wu M, Lei Y, MoS nanosheets with expanded interlayer spacing for enhanced sodium storage, Inorganic Chemistry Frontiers, 2018, 5, 3099-3105

Dong J, Zhang X, Huang J, Gao S, Mao J, Cai J, Chen Z, Sathasivam S, Carmalt CJ, Lai Y. Boosting heterojunction interaction in electrochemical construction of MoS_a quantum dots@TiO2 nanotube arrays for highly effective photoelectrochemical performance and electrocatalytic hydrogen evolution, Electrochemistry Communications, 2018, 93, 152-157

Dong Y, Xu Y, Li W, Fu Q, Wu M, Manske E, Kröger J, Lei Y, Insights into the Crystallinity of Layer-Structured Transition Metal Dichalcogenides on Potassium Ion Battery Performance: A Case Study of Molybdenum Disulfide, Small, 43542, 2019, 15, e1900497

Durndell LJ, Isaacs MA, Li C, Parlett CMA, Wilson K, Lee AF, Cascade Aerobic Selective Oxidation over Contiguous Dual-Catalyst Beds in Continuous Flow, ACS Catalysis, 2019, 9, 5345-5352

Eelen G, Dubois C, Cantelmo AR, Goveia J, Brüning U, DeRan M, Jarugumilli G, van Rijssel J, Saladino G, Comitani F, Zecchin A, Rocha S, Chen R, Huang H, Vandekeere S, Kalucka J, Lange C, Morales-Rodriguez F, Cruys B, Treps L, Ramer L, Vinckier S, Brepoels K, Wyns S, Souffreau J, Schoonjans L, Lamers WH, Wu Y, Haustraete J, Hofkens J, Liekens S, Cubbon R, Ghesquière B, Dewerchin M, Gervasio FL, Li X, van Buul JD, Wu X, Carmeliet P, Role of glutamine synthetase in angiogenesis beyond glutamine synthesis, Nature, 2018, 561, 63-69

Efthymiopoulos I, Hellier P, Ladommatos N, Russo-Profili A, Eveleigh A, Aliev AE, Kay A, Mills-Lamptey B, Influence of solvent selection and extraction temperature on yield and composition of lipids extracted from spent coffee grounds, Industrial Crops and Products, 2018, **119**, 49-56

Elmas S, Macdonald TJ, Skinner W, Andersson M, Nann T, Copper Metallopolymer Catalyst for the Electrocatalytic Hydrogen Evolution Reaction (HER), Polymers, 2019, 11, 110

Lee G, Che M, Qian E, Wang L, Gupta A, Neal R, Yue D, Downs S, Mayes T, Rose O, Acree WE Jr. and Abraham MH, Determination of Abraham model solute descriptors for o-acetoacetanisidide based on experimental solubility data in organic mono-solvents, Phys. Chem. Liquids, 2019, 57, 528-535

Fabian DM, Ganose AM, Ziller JW, Scanlon DO, Beard MC, Ardo S, Influence of One Specific Carbon-Carbon Bond on the Quality, Stability, and Photovoltaic Performance of Hybrid Organic-Inorganic Bismuth Iodide Materials, ACS Applied Energy Materials, 2019, 2, 1579-1587

Fielding HH, Henley A, Anion photoelectron spectroscopy of protein chromophores, International Reviews in Physical Chemistry, 2019, 38, 1-34

Finegan DP, Vamvakeros A, Cao L, Tan C, Heenan TMM, Daemi SR, Jacques SDM, Beale AM, Di Michiel M, Smith K, Brett DJL, Shearing PR, Ban C, Spatially Resolving Lithiation in Silicon-Graphite Composite Electrodes via in Situ High-Energy X-ray Diffraction Computed Tomography, Nano Letters, 2019, 19, 3811-3820

Firth FCN, Cliffe MJ, Vulpe D, Aragones-Anglada M, Moghadam PZ, Fairen-Jimenez D, Slater B, Grey CP, Engineering new defective phases of UiO family metal-organic frameworks with water, Journal of Materials Chemistry A, 2019, **7**, 7459-7469

Tsotinis A, Kompogennitaki R, Papanastasiou I, Garratt PJ, Bocianowska A, and Sugden D, Fluorine substituted methoxyphenylalkyl amides as potent melatonin receptor agonists Med. Chem, Commun. 2019, 10, 460

Foglia F, Hazael R, Meersman F, Wilding MC, Sakai VG, Rogers S, Bove LE, Koza MM, Moulin M, Haertlein M, Forsyth VT, McMillan PF, In Vivo Water Dynamics in Shewanella oneidensis Bacteria at High Pressure, Scientific Reports, 2019, 9, 8716

Forte N, Chudasama V, Baker JR, Homogeneous antibody-drug conjugates via site-selective disulfide bridging, Drug Discovery Today: Technologies, 2018, **30**. 011-20

Galan SRG, Wickens JR, Dadova J, Ng W-L, Zhang X, Simion RA, Quinlan R, Pires E, Paton RS, Caddick S, Chudasama V, Davis BG, Posttranslational site-selective protein backbone α-deuteration, Nature Chemical Biology, 2018, 14, 955-963

Galdadas I, Lovera S, Pérez-Hernández G, Barnes MD, Healy J, Afsharikho H, Woodford N, Bonomo RA, Gervasio FL, Haider S, Defining the architecture of KPC-2 Carbapenemase: identifying allosteric networks to fight antibiotics resistance, Scientific Reports, 2018, 8, 12916

Gardecka AJ, Lübke M, Armer CF, Ning D, Reddy MV, Williams AS, Lowe A, Liu Z, **Parkin IP**, **Darr JA**, Nb-doped rutile titanium dioxide nanorods for lithium-ion batteries, *Solid State Sciences*, 2018, **83**, 115-121

Gendron T, Sander K, Cybulska K, Benhamou L, Sin PKB, Khan A, Wood M, **Porter MJ**, **Årstad E**, Ring-Closing Synthesis of Dibenzothiophene Sulfonium Salts and Their Use as Leaving Groups for Aromatic 18F-Fluorination, *Journal* of the American Chemical Society, 2018, **140**, 11125-11132

Gherghel S, Morgan RM, Arrebola-Liébanas JF, **Blackman CS**, **Parkin IP**, Fragrance transfer between fabrics for forensic reconstruction applications, *Science and Justice*, 2019, **59**, 256-2677

Giussani A, **Worth GA**, Similar chemical structures, dissimilar triplet quantum yields: a CASPT2 model rationalizing the trend of triplet quantum yields in nitroaromatic systems, *Physical Chemistry Chemical Physics*, 2019, **21**, 10514-10522

Sedov A, Magsumov TI, Hart E, Ramirez A M, Cheeran S, Barrera M, Horton MY, Wadawadigi A, Zha O, Tong XY, Acree WE Jr, and **Abraham MH**, Abraham model correlations for triethylene glycol solvent derived from infinite dilution activity coefficient, partition coefficient and solubility data measured at 298.15 *K, J. Soln. Chem.*, 2017, 46, 2249-2267

Greenwood HE, McCormick PN, Gendron T, Glaser M, Pereira R, Maddocks ODK, **Sander K**, Zhang T, Koglin N, Lythgoe MF, **Årstad E**, Hochhauser D, Witney TH, Measurement of tumor antioxidant capacity and prediction of chemotherapy resistance in preclinical models of ovarian cancer by positron emission tomography, *Clinical Cancer Research*, 2019, **25**, 2471-2482

Greer AJ, Taylor SFR, Daly H, Quesne M, Catlow CRA, Jacquemin J, Hardacre C, Investigating the Effect of NO on the Capture of CO₂ Using Superbase Ionic Liquids for Flue Gas Applications, ACS Sustainable Chemistry and Engineering, 2019, 7, 3567-3574

Griffin M, **Palgrave R**, Baldovino-Medrano V, Butler PE, Kalaskar DM, Argon plasma improves the tissue integration and angiogenesis of subcutaneous implants by modifying surface chemistry and topography, *International Journal of Nanomedicine*, 2018, **13**, 6123-6141

Groen D, Richardson RA, Wright DW, Jancauskas V, Sinclair R, Karlshoefer P, Vassaux M, Arabnejad H, Piontek T, Kopta P, Bosak B, Lakhlili J, Hoenen O, Suleimenova D, Edeling W, Crommelin D, Nikishova A, **Coveney PV**, Introducing VECMAtk - Verification, Validation and Uncertainty Quantification for Multiscale and HPC Simulations, *Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics)*, 2019, **11539**, 479-492

Gusken NA, Lauri A, Li Y, Matsui T, Doiron B, Bower R, **Regoutz A**, Mihai A, Petrov PK, Oulton RF, Cohen LF, Maier SA, TiO₂-x-Enhanced IR Hot Carrier Based Photodetection in Metal Thin Film-Si Junctions, *ACS Photonics*, 2019, **6**, 953-960

Hager R, Arnold A, Sevcsik E, Schütz GJ, **Howorka S**, Tunable DNA Hybridization Enables Spatially and Temporally Controlled Surface-Anchoring of Biomolecular Cargo, *Langmuir*, 2018, **34**, 15021-15027

Hailes HC, Subrizi F, Benhamou L, Ward J, Sheppard TD, Aminopolyols from carbohydrates: the amination of sugars and sugar-derived tetrahydrofurans with transaminases, *Angewandte Chemie - International Edition*, 2019, **58**, 3854-3858

Hailes HC, Ward JM, Wang Y, Tappertzhofen N, Mendez-Sanchez D, Bawn M, Lyu B, Design and use of de novo cascades for new benzylisoquinoline alkaloid biosynthesis, *Angewandte Chemie International Edition*, 2019, **58**, 10120-10125

Haldar S, Comitani F, Saladino G, Woods C, van der Kamp MW, Mulholland AJ, **Gervasio FL**, A Multiscale Simulation Approach to Modeling Drug-Protein Binding Kinetics, *Journal of Chemical Theory and Computation*, 2018, **14**, 6093-6101

Harman CLG, Patel MA, Guldin S, **Davies G-L**, Recent developments in Pickering emulsions for biomedical applications, *Current Opinion in Colloid & Interface Science*, 2019, **39**, 173-189

Hart M, Chen J, Michaelides A, **Sella A**, Shaffer MSP, **Salzmann CG**, One-Dimensional Arsenic Allotropes: Polymerization of Yellow Arsenic Inside Single-Wall Carbon Nanotubes, *Angewandte Chemie International Edition*, 2018, **57**, 11649-11653

Hasnain SS, **Catlow CRA**, Synchrotron science in the UK: NINA, the SRS and Diamond, *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 2019, **377**, 20190147

He G, Han X, Moss B, Weng Z, Gadipelli S, Lai F, Kafizas AG, Brett DJL, **Guo ZX**, Wang H, **Parkin IP**, Solid solution nitride/ carbon nanotube hybrids enhance electrocatalysis of oxygen in zinc-air batteries, *Energy Storage Materials*, 2018, **15**, 380-387

Heath-Apostolopoulos I, Wilbraham L, **Zwijnenburg M**, Computational High-Throughput Screening of Polymeric Photocatalysts: Exploring the Effect of Composition, Sequence Isomerism and Conformational Degrees of Freedom, *Faraday Discussions*, 2018, **215**, 98-110

Henley A, Patel AM, Parkes MA, Anderson JC, **Fielding HH**, The Role of Photoisomerisation on the Photodetachment of the Photoactive Yellow Protein Chromophore, *Journal of Physical Chemistry A*, 2018, **122**, 8222-8228

Ho-Kimura S, Williamson BAD, Sathasivam S, Moniz SJA, He G, Luo W, **Scanlon DO**, Tang J, **Parkin IP**, Origin of High-Efficiency Photoelectrochemical Water Splitting on Hematite/Functional Nanohybrid Metal Oxide Overlayer Photoanode after a Low Temperature Inert Gas Annealing Treatment, *ACS Omega*, 2019, **4**, 1449-1459

Kamble S, Loadman P, **Abraham, MH**, and Liu X, Structural properties governing drug- plasma protein binding determined by high-performance liquid chromatography method, *J. Pharm. Biomed. Analysis*, 2018, **149**, 16-21

Lu JZ, Acree WE Jr, and **Abraham MH**, Updated Abraham model correlations for enthalpies of solvation of organic solutes dissolved in benzene and acetonitrile, *Phys. Chem. Liquids*, 2018, **57**, 84-99

Hodgkins TL, Savory CN, Bass KK, Seckman BL, **Scanlon DO**, Djurovich PI, Thompson ME, Melot BC, Anionic order and band gap engineering in vacancy ordered triple perovskites, *Chemical Communications*, 2019, **55**, 3164-3167

Hoekstra AG, Chopard B, Coster D, Zwart SP, **Coveney PV**, Multiscale computing for science and engineering in the era of exascale performance, Philosophical Transactions of the Royal Society A: Mathematical, *Physical and Engineering Sciences*, 2019, **377**, 20180144

Hoekstra AG, Zwart SP, Coveney PV, Multiscale modelling, simulation and computing: From the desktop to the exascale, *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 2019, **377**, 20180355

PUBLICATIONS

Hou Q, Buckeridge J, Lazauskas T, Mora-Fonz D, Sokol AA, Woodley SM, Catlow CRA, Defect formation in In O. and SnO₂: a new atomistic approach based on accurate lattice energies, Journal of Materials Chemistry C, 2018, **6**, 12386-12395

Hovan L, Comitani F, Gervasio FL, Defining an Optimal Metric for the Path Collective Variables, Journal of Chemical Theory and Computation, 2019, 15, 25-32

Hu D, Zhao T, Ping X, Zheng H, Xing L, Liu X, Zheng J, Sun L, Gu L, Tao C, Wang D, Jiao L, Unveiling the Layer-Dependent Catalytic Activity of PtSe <inf>2</inf> Atomic Crystals for the Hydrogen Evolution Reaction, Angewandte Chemie - International Edition English, 2019, 58, 6977-6981

Hu L, Johnson ID, Kim S, Nolis GM, Freeland JW, Yoo HD, Fister TT, McCafferty L, Ashton TE, Darr JA, Cabana J, Tailoring the electrochemical activity of magnesium chromium oxide towards Mg batteries through control of size and crystal structure, Nanoscale, 2019, **11**, 639-646

Humphrey DS, Pang CL, Chen Q, Thornton G, Electron induced nanoscale engineering of rutile TiO₂ surfaces, Nanotechnology, 2019, 30, 025303

Hussain H, Ahmed MHM, Torrelles X, Grinter DC, Cabailh G, Bikondoa O, Nicklin C, Aschauer U, Lindsay R, Thornton G, Water-Induced Reversal of the $TiO_0(011)$ -(2 × 1) Surface Reconstruction: Observed with in Situ Surface X-ray Diffraction, Journal of Physical Chemistry C, 2019, 123, 13545-13550

Isaacs MA, Robinson N, Barbero B, Durndell LJ, Manayil JC, Parlett CMA, D'Agostino C, Wilson K, Lee AF, Unravelling mass transport in hierarchically porous catalysts, Journal of Materials Chemistry A, 2019, 7, 11814-11825

luzzolino L, McCabe P, Price SL, Brandenburg JG, Crystal structure prediction of flexible pharmaceutical-like molecules: Density functional tightbinding as an intermediate optimization method and for free energy estimation, Faraday Discussions, 2018, 211, 275-296

Jabłońska M, Arán MA, Beale AM, Delahay G, Petitto C, Nocuń M, Palkovits R, Understanding the origins of N₂O ecomposition activity in Mn(Fe)CoAlO hydrotalcite derived mixed metal oxides, Applied Catalysis B: Environmental, 2019, 243, 66-75

Jabłońska M, Arán MA, Beale AM, Góra-Marek K, Delahay G, Petitto C, Pacultová K, Palkovits R, Catalytic decomposition of N₂O over Cu-Al-O₂ mixed metal oxides, RSČ Advances, 2019, 9, 3979-3986

Jabłońska M, Beale AM, Nocuń M, Palkovits R, Ag-Cu based catalysts for the selective ammonia oxidation into nitrogen and water vapour, Applied Catalysis B: Environmental, 2018, 232, 275-287

Jaiswal N, Pandey CM, Soni A, Tiwari I, Rosillo-Lopez M, Salzmann CG, Malhotra BD, Sumana G, Electrochemical genosensor based on carboxylated graphene for detection of water-borne pathogen, Sensors and Actuators, B: Chemical, 2018, 275, 312-321

Janicki MJ, Roberts SJ, Šponer J, Powner MW, Góra RW, Szabla R, Photostability of oxazoline RNA-precursors in UV-rich prebiotic environments., Chemical Communications, 2018, 54, 13407-13410

Jenkins AJ, Spinlove KE, Vacher M, Worth GA, Robb MA, The Ehrenfest method with fully quantum nuclear motion (Qu-Eh): Application to charge migration in radical cations, Journal of Chemical Physics, 2018, 149, 94108

Jia J, White ER, Clancy AJ, Rubio Carrero N, Suter T, Miller TS, McMillan PF, Brázdová V, Corà F, Howard CA, Mattevi C, Shaffer M, Fast Exfoliation and Functionalisation of 2D Crystalline Carbon Nitride by Framework Charging, Angewandte Chemie International Edition, 2018, 57, 12656-12660

Jolly P, Rainbow J, Regoutz A, Estrela P, Moschou D, A PNA-based Lab-on-PCB diagnostic platform for rapid and high sensitivity DNA quantification, Biosensors & Bioelectronics, 2019, 123, 244-250

Jurcic M, Peveler WJ, Savory CN, Bučar D-K, Kenyon AJ, Scanlon DO, Parkin IP, Sensing and Discrimination of Explosives at Variable Concentrations with a Large-Pore MOF as Part of a Luminescent Array, ACS Applied Materials & Interfaces, 2019, 11, 11618-11626

Kammert JD, Xie J, Godfrey IJ, Unocic RR, Stavitski E, Attenkofer K, Sankar G, Davis RJ, Reduction of Propionic Acid over a Pd-Promoted ReO /SiO Catalyst Probed by X-ray Absorption Spectroscopy and Transient Kinetic Analysis, ACS Sustainable Chemistry and Engineering, 2018, 6, 12353-12366 Kampouri S, Nguyen TN, Spodaryk M, Palgrave RG, Züttel A, Smit B, Stylianou KC, Concurrent Photocatalytic Hydrogen Generation and Dye Degradation Using MIL-125-NH, under Visible Light Irradiation, Advanced Functional Materials, 2018, 28, 1806368

Karmaoui M, Jorge AB, McMillan PF, Aliev AE, Pullar RC, Labrincha JA, Tobaldi DM, One-Step Synthesis, Structure, and Band Gap Properties of SnO Nanoparticles Made by a Low Temperature Nonaqueous Sol-Gel Technique, ACS Omega, 2018, 3, 13227-13238

Karthick Kannan P, Shankar P, Blackman C, Chung CH, Recent Advances in 2D Inorganic Nanomaterials for SERS Sensing, Advanced Materials, 2019, 31, 1803432

Karthikeyan S, Jo WK, Dhanalakshmi R, Isaacs MA, Wilson K, Sekaran G, Lee AF, A porous activated carbon supported Pt catalyst for the oxidative degradation of poly[(naphthaleneformaldehyde) sulfonate], Journal of the Taiwan Institute of Chemical Engineers, 2018, 93, 289-297

Karthikeyan S, Kumar S, Durndell LJ, Isaacs MA, Parlett CMA, Coulson B, Douthwaite RE, Jiang Z, Wilson K, Lee AF, Size-Dependent Visible Light Photocatalytic Performance of Cu₂O Nanocubes, ChemCatChem, 2018, 10, 3554-3563

Khan J, Liu Y, Zhao T, Geng H, Xu W, Shuai Z, High performance thermoelectric materials based on metal organic coordination polymers through firstprinciples band engineering, Journal of Computational Chemistry, 2018, 39, 2582-2588

Knapp CE, Metcalf EA, Mrig S, Sanchez-Perez C, Douglas SP, Choquet P, Boscher ND, Precursors for Atmospheric Plasma-Enhanced Sintering: Low-Temperature Inkjet Printing of Conductive Copper, ChemistryOpen, 2018, 7, 850-857

Kudsiova L, Mohammadi A, Mustapa MFM, Campbell F, Welser K, Vlaho D, Story H, Barlow DJ, Tabor AB, Hailes HC, Lawrence MJ, Trichain cationic lipids: the potential of their lipoplexes for gene delivery, Biomaterials Science, 2019, 7, 149-158

Kuzmanic A, Pritchard RB, Hansen DF, Gervasio FL, Importance of the Force Field Choice in Capturing Functionally Relevant Dynamics in the von Willebrand Factor, Journal of Physical Chemistry Letters, 2019, 10, 1928-1934

Larocca M, **Foglia F**, Cilibrizzi A, Dihedral Angle Calculations To Elucidate the Folding of Peptides through Its Main Mechanical Forces, Biochemistry, 2019, **58**, 1032-1037

Laserna V, Jeapes Rojas C, **Sheppard TD**, Gold-Catalyzed Hydrophenoxylation of Propargylic Alcohols and Amines: Synthesis of Phenyl Enol Ethers, *Organic Letters*, 2019, **21**, 4443-4447

Lee W-C, Wahila MJ, Mukherjee S, Singh CN, Eustance T, **Regoutz A**, Paik H, Boschker JE, Rodolakis F, Lee T-L, Schlom DG, Piper LFJ, Cooperative effects of strain and electron correlation in epitaxial VO₂ and NbO₂, *Journal of Applied Physics*, 2019, **125**, 082539

Lee WJ, **Clancy AJ**, Fernández-Toribio JC, Anthony DB, White ER, Solano E, Leese HS, Vilatela JJ, Shaffer MSP, Interfacially-grafted single wall carbon nanotube / poly (vinyl alcohol) composite fibers, *Carbon*, 2019, **146**, 162-171

Leipold L, Dobrijevic D, Jeffries J, Bawn M, Moody T, Ward J, **Hailes HC**, The identification and use of robust transaminases from a domestic drain metagenome, *RSC Green Chemistry*, 2019, **21**, 75-86

Leung WWW, Savory CN, **Palgrave RG**, **Scanlon DO**, An experimental and theoretical study into NaSbS₂ as an emerging solar absorber, *Journal of Materials Chemistry C*, 2019, **7**, 2059-2067

Li J, Sathasivam S, Taylor A, **Carmalt CJ**, **Parkin IP**, Single step route to highly transparent, conductive and hazy aluminium doped zinc oxide films, *RSC Advances*, 2018, **8**, 42300-42307

Li L, **Slater B**, Yan Y, Wang C, Li Y, Yu J, Necessity of heteroatoms for realizing hypothetical aluminophosphate zeolites: A high-throughput computational approach, *Journal of Physical Chemistry Letters*, 2019, **10**, 1411-1415

Li S, Page K, Sathasivam S, Heale F, He G, Lu Y, Lai Y, Chen G, **Carmalt CJ**, **Parkin IP**, Efficiently texturing hierarchical superhydrophobic fluoridefree translucent films by AACVD with excellent durability and self-cleaning ability, *Journal of Materials Chemistry A*, 2018, **6**, 17633-1764

Li T, Heenan TMM, Rabuni MF, Wang B, Farandos NM, Kelsall GH, Matras D, Tang C, Lu X, Jacques SDM, Brett DJL, Shearing PR, Di Michiel M, **Beale AM**, Vamvakeros A, Li K, Design of nextgeneration ceramic fuel cells and real-time characterization with synchrotron X-ray diffraction computed tomography, *Nature Communications*, 2019, **10**, 1497

Hart E, Klein A, Barrera M, Jodray M, Rodriguez K, Acree WE Jr, and **Abraham MH**, Development of Abraham model correlations for describing the transfer of molecular solutes into propanenitrile and butanenitrile from water and from the gas phase, *Physics Chem.Liquids*, 2018, 56, 821-833

Li W, **Xu Y**, Dong Y, Wu Y, Zhang C, Zhou M, Fu Q, Wu M, Lei Y, Bismuth oxychloride nanoflake assemblies as a new anode for potassium ion batteries, *Chemical Communications*, 2019, **55**, 6507-6510

Ling M, **Blackman CS**, Gas-phase synthesis of hybrid nanostructured materials, *Nanoscale*, 2018, **10**, 22981-22989

Liu L, Chen Z, Wang J, Zhang D, Zhu Y, Ling S, Huang KW, Belmabkhout Y, Adil K, Zhang Y, **Slater B**, Eddaoudi M, Han Y, Imaging defects and their evolution in a metal–organic framework at sub-unit-cell resolution, *Nature Chemistry*, 2019, **11**, 622-628

Liu Y, Shi W, **Zhao T**, Wang D, Shuai Z, Boosting the Seebeck Coefficient for Organic Coordination Polymers: Role of Doping-Induced Polaron Band Formation, Journal of Physical Chemistry Letters, 2019, **10**, 2493-2499

Loe R, Huff K, Walli M, Morgan T, Qian D, Pace R, Song Y, **Isaacs M**, Santillan-Jimenez E, Crocker M, Effect of Pt Promotion on the Ni-Catalyzed Deoxygenation of Tristearin to Fuel-Like Hydrocarbons, *Catalysts*, 2019, **9**, 200

Logsdail AJ, Downing CA, Keal TW, Sherwood P, Sokol AA, **Catlow CRA**, Hybrid-DFT Modeling of Lattice and Surface Vacancies in MnO, *Journal of Physical Chemistry C*, 2019, **123**, 8133-8144

Lu H, Andrei V, Jenkinson K, **Regoutz A**, Li N, Creissen CE, Wheatley AEH, Hao H, Reisner E, Wright DS, Pike SD, Single-Source Bismuth (Transition Metal) Polyoxovanadate Precursors for the Scalable Synthesis of Doped BiVO4 Photoanodes, *Advanced Materials*, 2018, **30**, 1804033

Lu Y, Farrow MR, Fayon P, Logsdail AJ, Sokol AA, **Catlow CRA**, Sherwood P, Keal TW, Open-Source, Python-Based Redevelopment of the ChemShell Multiscale QM/MM Environment, *Journal* of Chemical Theory and Computation, 2019, **15**, 1317-1328 Luo L, Zhang Q, Luo Y, He Z, Tian X, **Battaglia G**, Thermosensitive nanocomposite gel for intra-tumoral two-photon photodynamic therapy, *Journal of Control Release*, 2019, **298**, 99-109 **Macdonald TJ**, Ambroz F, Batmunkh M, Li Y, Kim D, Contini C, Poduval R, Liu H, Shapter JG, Papakonstantinou I, **Parkin IP**, TiO₂ nanofiber photoelectrochemical cells loaded with sub-12 nm AuNPs: Size dependent performance evaluation, *Materials Today Energy*, 2018, **9**, 254-263

Malarde D, Johnson I, Godfrey I, Powell M, Cibin G, Quesada Cabrera R, **Darr JA**, **Carmalt CJ**, **Sankar G**, **Parkin IP**, **Palgrave RG**, Direct and Continuous Hydrothermal Flow Synthesis of Thermochromic Phase Pure Monoclinic VO₂ Nanoparticles, *Journal of Materials Chemistry C*, 2018, **6**, 11731-11739

Marin-Beloqui JM, Fallon KJ, Bronstein H, Clarke TM, Discerning Bulk and Interfacial Polarons in a Dual Electron Donor/ Acceptor Polymer, *Journal of Physical Chemistry Letters*, 2019, **10**, 3813-3819

Maruani A, Bispecifics and antibody—drug conjugates: A positive synergy, *Drug Discovery Today: Technologies*, 2018, **30**, 55-61

Matam SK, Howe RF, Thetford A, **Catlow CRA**, Room temperature methoxylation in zeolite H-ZSM-5: an operando DRIFTS/mass spectrometric study, *Chemical Communications*, 2018, **54**, 12875-12878

Matras D, Jacques SDM, Poulston S, Grosjean N, Estruch Bosch C, Rollins B, Wright J, Di Michiel M, Vamvakeros A, Cernik RJ, **Beale AM**, Operando and Postreaction Diffraction Imaging of the La-Sr/CaO Catalyst in the Oxidative Coupling of Methane Reaction, *Journal of Physical Chemistry C*, 2019, **123**, 1751-1760

Mattedi G, Deflorian F, Mason JS, de Graaf C, **Gervasio FL**, Understanding ligand binding selectivity in a prototypical GPCR family., *Journal of Chemical Information and Modeling*, 2019, **59**, 2830-2836

Maughan AE, Ganose AM, **Scanlon DO**, Neilson JR, Perspectives and Design Principles of Vacancy-Ordered Double Perovskite Halide Semiconductors, *Chemistry of Materials*, 2019, **31**, 1184-1195

Mazibuko AF, Chauke HR, Ngoepe PE, Catlow CRA, Interatomic potential parameters for Li-Cl-Ti interaction, *IOP Conference Series: Materials Science and Engineering*, 2018, **430**, 012016

McColl K, Corà F, Mg2+ storage and mobility in anatase TiO2: the role of frustrated coordination, Journal of Materials Chemistry A, 2019, 7, 3704-3713

McColl K, Corà F, Phase stability of intercalated V₂O₂ battery cathodes elucidated through the Goldschmidt tolerance factor, Physical Chemistry Chemical Physics, 2019, 21, 7732-7744

McCormick PN, Greenwood HE, Glaser M, Maddocks ODK, Gendron T, Sander K, Gowrishankar G, Hoehne A, Zhang T, Shuhendler AJ, Lewis DY, Berndt M, Koglin N, Lythgoe MF, Gambhir SS, Arstad E, Witney TH, Assessment of tumor redox status through (S)-4-(3-[18F] fluoropropyl)-L-glutamic acid positron emission tomography imaging of system xc- activity, Cancer Research, 2018, 79, 853-863

McMillan PF, New nitrides: from high pressure-high temperature synthesis to layered nanomaterials and energy applications, Philosophical Transactions A: Mathematical, Physical and Engineering Sciences, 2019, 377, 0244

Mielewczyk-Gryń A, Wachowski S, Prześniak-Welenc M, Dzierzgowski K, Regoutz A, Payne DJ, Gazda M, Water uptake analysis of acceptor-doped lanthanum orthoniobates, Journal of Thermal Analysis and Calorimetry, 2019, 1-8

Mitchell SA, Truscott F, Dickman R, Ward J, Tabor AB, Simplified lipid IIbinding antimicrobial peptides: Design, synthesis and antimicrobial activity of bioconjugates of nisin rings A and B with pore-forming peptides, Bioorganic and Medicinal Chemistry, 2018, 26, 5691-5700

Mohammadi A, Kudsiova L, Mustapa MFM, Campbell F, Vlaho D, Welser K, Story H, Tagalakis AD, Hart SL, Barlow DJ, Tabor AB, Lawrence MJ, Hailes HC, The discovery and enhanced properties of trichain lipids in lipopolyplex gene delivery systems, Organic & Biomolecular Chemistry, 2019, 17, 945-957

Morozov IG, Sathasivam S, Belousova OV, Parkin IP, Kuznetcov MV, Effect of synthesis conditions on room-temperature ferromagnetic properties of Mg-O nanoparticles, Journal of Alloys and Compounds, 2018, 765, 343-354

Nair HS, Kumar CMN, Adroja DT, Ritter C, Wills AS, Kockelmann WA, Deen PP, Bhattacharyya A, Strydom AM, Magnetic structure and field-dependent magnetic phase diagram of Ni2In-type PrCuSi, Journal of Physics-Condensed Matter, 2018, 30, 435803

Nastase SAF, O'Malley AJ, Catlow CRA, Logsdail AJ, Computational QM/MM investigation of the adsorption of MTH active species in H-Y and H-ZSM-5, Physical Chemistry Chemical Physics, 2019, 21, 2639-2650

Nguyen HP, Stewart S, Kukwikila MN, Jones SF, Offenbartl-Stiegert D, Mao S, Balasubramanian S, Beck S, Howorka S, Opto-epigenetic modulation of DNA methylation with a photo-responsive small-molecule approach, Angewandte Chemie - International Edition English, 2019, 58, 6620-6624

Nogueira JCF, Greene MK, Richards DA, Furby AO, Steven J, Porter A, Barelle C, Scott CJ, Chudasama V, Oriented attachment of VNAR proteins, via siteselective modification, on PLGA-PEG nanoparticles enhances nanoconiugate performance, Chemical Communications, 2019, **55**, 7671-7674

Offenbartl-Stiegert D, Clarke TM, Bronstein H, Nguyen HP, Howorka S, Solvent-dependent photophysics of a red-shifted, biocompatible coumarin photocage, Organic & Biomolecular Chemistry, 2019, 17, 6178-6183

Oliveira Lourenco CR, Macdonald TJ, Gavriilidis A, Allan E, Macrobert A, Parkin IP, Effects of bovine serum albumin on light activated antimicrobial surfaces, RSC Advances, 2018, 8, 3452-3458

Ordan M, Pallara C, Maik-Rachline G, Hanoch T, Gervasio FL, Glaser F, Fernandez-Recio J, Seger R, Intrinsically active MEK variants are differentially regulated by proteinases and phosphatases, Scientific Reports, 2018, 8, 11830

Palmer RA, Lisgarten DR, Cockcroft JK, Lisgarten JN, Talbert R, Dines T, Bansal R, Acharya PC, Suryan A, Crystal and Molecular Structure and DFT Calculations of the Steroidal Oxime 6E-Hydroximinoandrost-4-ene-3,17-dione (C19H25NO3) a Molecule with Antiproliferative Activity. Journal of Chemical Crystallography, 2019, 49, 29-36

Papineau D, DeGregorio B, Sagar J, Thorogate R, wang J, Nittler L, Kilcoyne D, Marbach H, Drost M, Thornton G, Fossil biomass preserved as graphitic carbon in a late Paleoproterozoic banded iron formation metamorphosed at more than 550oC, Journal of the Geological Society of London, 2019, 176, 651-668

Parkes M, Bennett A, Fielding HH, A photoelectron imaging and quantum chemistry study of the deprotonated cvan fluorescent protein chromophore anion, Molecular Physics, 2018, 20, 15543-15549

Parkes M, Douglas K, Price SD, Ionization of Acetonitrile, International Journal of Mass Spectrometry, 2019, 438, 97-106

Paterson AF, Singh S, Fallon KJ, Hodsden T, Han Y, Schroeder BC, Bronstein H, Heeney M, McCulloch I, Anthopoulos TD. Recent Progress in High-Mobility Organic Transistors: A Reality Check, Advanced Materials, 2018, **30**, 1801079

Patrick PS, Bogart LK, Macdonald TJ, Southern P, Powell MJ, Zaw-Thin M, Voelcker NH, Parkin IP, Pankhurst QA, Lythgoe MF, Kalber TL, Bear JC, Surface radio-mineralisation mediates chelate-free radiolabelling of iron oxide nanoparticles, Chemical Science, 2019, **10**, 2592-2597

Pegg JT, Shields AE, Storr MT, **Scanlon** DO, De Leeuw NH, Noncollinear Relativistic DFT + U Calculations of Actinide Dioxide Surfaces, Journal of Physical Chemistry C, 2019, 123, 356-366

Pegg JT, Shields AE, Storr MT, Scanlon DO, de Leeuw NH, Interaction of hydrogen with actinide dioxide (111) surfaces, Journal of Chemical Physics, 2019, **150**, 134701

Pegg JT, Shields AE, Storr MT, Wills AS, Scanlon DO, de Leeuw NH, Hidden magnetic order in plutonium dioxide nuclear fuel, Physical Chemistry Chemical Physics, 2018, 20, 20943-20951

Pegg JT, Shields AE, Storr MT, Wills AS, Scanlon DO, de Leeuw NH, Magnetic structure of UO, and NpO, by first-principle methods, Physical Chemistry Chemical Physics, 2019, 21, 761-770

Pereira R, Gendron T, Sanghera C, Greenwood HE, Newcombe J, McCormick P, Sander K, Topf M, Arstad E, Witney TH, Mapping Aldehyde Dehydrogenase 1A1 Activity using an [18F]Substratebased Approach, Chemistry, 2019, 25, 2345-2351

Perera AS, Cockcroft JK, Trogadas P, Yu H, Kapil N, Coppens MO, Titanium(IV)-induced cristobalite formation in titanosilicates and its potential impact on catalysis, Journal of Materials Science, 2019, 54, 335-345

Perez Garcia L, Donlucas Perez J, Volpe ${\bf G}$, Arzola AV, Volpe G, High-performance reconstruction of microscopic force fields from Brownian trajectories, Nature Communications, 2018, 9, 5166

Peveler WJ, Jia H, Jeen T, Rees K, **Macdonald TJ**, Xia Z, Chio W-lK, Moorthy S, **Parkin IP**, **Carmalt CJ**, Algar WR, Lee T-C, Cucurbituril-mediated quantum dot aggregates formed by aqueous self-assembly for sensing applications, *Chemical Communications*, 2019, **55**, 5495-5498

Peveler WJ, Packman H, Alexander S, Chauhan RR, Hayes LM, **Macdonald TJ**, **Cockcroft JK**, Rogers S, Aarts DGAL, **Carmalt CJ**, **Parkin IP**, Bear JC, A new family of urea-based low molecularweight organogelators for environmental remediation: the influence of structure, *Soft Matter*, 2018, **14**, 8821-8827

Phillips LJ, Savory CN, Hutter OS, Yates PJ, Shiel H, Mariotti S, Bowen L, Birkett M, Durose K, **Scanlon DO**, Major JD, Current Enhancement via a TiO₂ Window Layer for CSS Sb2Se3 Solar Cells: Performance Limits and High Voc, *IEEE Journal of Photovoltaics*, 2019, **9**, 544-551

Playford HY, Whale TF, Murray B, Tucker MG, **Salzmann CG**, Analysis of stacking disorder in ice I using pair distribution functions, *Journal of Applied Crystallography*, 2018, **51**, 1211-1220

Ploszajski AR, Billing M, **Cockcroft JK**, Skipper NT, Crystalline structure of an ammonia borane-polyethylene oxide cocrystal: a material investigated for its hydrogen storage potential, *CrystEngComm*, 2018, **20**, 4436-4440

Ploszajski AR, Billing M, Skipper NT, **Cockcroft JK**, A novel ammonium pentaborate – poly(ethylene-glycol) templated polymer-inclusion compound, *Chemical Communications*, 2019, **55**, 8290-8292

Pont S, Foglia F, Higgins AM, **Durrant JR**, Cabral JT, Stability of Polymer:PCBM Thin Films under Competitive Illumination and Thermal Stress, *Advanced Functional Materials*, 2018, **28**, 1802520

Potter DB, **Parkin IP**, **Carmalt CJ**, The effect of solvent on Al-doped ZnO thin films deposited via aerosol assisted CVD, *RSC Advances*, 2018, **8**, 33164-33173

Potterton A, Husseini FS, Southey MW, Bodkin MJ, Heifetz A, **Coveney PV**, Townsend-Nicholson A, Ensemble-Based Steered Molecular Dynamics Predicts Relative Residence Time of A2A Receptor Binders, *Journal of Chemical Theory and Computation*, 2019, **15**, 3316-3330 Powell MJ, Williamson BAD, Baek SY, Manzi J, Potter DB, **Scanlon DO**, **Carmalt CJ**, Phosphorus doped SnO₂ thin films for transparent conducting oxide applications: synthesis, optoelectronic properties and computational models, *Chemical Science*, 2018, **9**, 7968-7980

Powner M, Ashe K, Fernandez Garcia C, Coggins A, Corpinot M, **Bučar D-K**, Selective prebiotic synthesis of phosphoroaminonitriles and aminothioamides inneutral water, *Communications Chemistry*, 2019, **2**, 23

Powner M, Whitaker D, Aponte JC, Elsila JE, Dworkin JP, Analyses of Aliphatic Aldehydes and Ketones in Carbonaceous Chondrites, *ACS Earth Space and Chemistry*, 2019, **3**, 463-472

Powner MW, Islam S, Protocells realize their potential, *Nature Catalysis*, 2018, 1, 569-570

Powner MW, Roberts S, Stairs S, **Bucar D**, Szabla R, Todd Z, Šponer J, Sasselov DD, Selective prebiotic conversion of pyrimidine and purine anhydronucleosides into Watson-Crick base-pairing arabino-furanosyl nucleosides in water, *Nature Communications*, 2018, **9**, 4073

Powner MW, Whitaker D, Prebiotic nucleic acids need space to grow, *Nature Communications*, 2018, **9**, 5172

Price S, Stevenson EL, Lancaster RW, Buanz ABM, **Price SL**, The solid state forms of the sex hormone 17-β-estradiol, *CrystEngComm*, 2019, **13**, 2154-2163

Price SL, Control and prediction of the organic solid state: a challenge to theory and experiment, *Proceedings of the Royal Society A - Mathematical Physical and Engineering Sciences*, 2018, **474**, 20180351

Price SWT, Van Loon A, Keune K, Parsons AD, Murray C, **Beale AM**, Mosselmans JFW, Unravelling the spatial dependency of the complex solid-state chemistry of Pb in a paint micro-sample from Rembrandt's Homer using XRD-CT, *Chemical Communications*, 2019, **55**, 1931-1934

Qin Y, Han X, Gadipelli S, Guo J, Wu S, Kang L, Callison J, **Guo Z**, In situ synthesized low-PtCo@porous carbon catalyst for highly efficient hydrogen evolution, *Journal of Materials Chemistry A*, 2019, **7**, 6543-6551

Quesne MG, Roldan A, De Leeuw NH, **Catlow CRA**, Carbon dioxide and water co-adsorption on the low-index surfaces of TiC, VC, ZrC and NbC: A DFT study, *Physical Chemistry Chemical Physics*, 2019, **21**, 10750-10760

Quesne MG, Silveri F, de Leeuw NH, Catlow CRA, Advances in sustainable catalysis: A computational perspective, *Frontiers in Chemistry*, 2019, **7**, 182

Raja FNS, Worthington T, Isaacs MA, Forto Chungong L, Burke B, Addison O, Martin RA, The Antimicrobial Efficacy of Hypoxia Mimicking Cobalt Oxide Doped Phosphate-Based Glasses against Clinically Relevant Gram Positive, Gram Negative Bacteria and a Fungal Strain, ACS Biomaterials Science and Engineering, 2019, 5, 283-293 Regoutz A, Ganose AM, Blumenthal L, Schlueter C, Lee TL, Kieslich G, Cheetham AK, Kerherve G, Huang YS, Chen RS, Vinai G, Pincelli T, Panaccione G, Zhang KHL, Egdell RG, Lischner J, Scanlon DO, Payne DJ, Insights into the electronic structure of OsO2 using soft and hard x-ray photoelectron spectroscopy in combination with density functional theory, Physical Review Materials, 2019, 3, 025001

Regoutz A, Kerherve G, Villar-Garcia I, Williams CK, Payne DJ, The influence of oxygen on the surface interaction between CO2 and copper studied by ambient pressure X-ray photoelectron spectroscopy, *Surface Science*, 2018, **677**, 121-127

Regoutz A, Pobegen G, Aichinger T, Interface chemistry and electrical characteristics of 4H-SiC/SiO2 after nitridation in varying atmospheres, *Journal of Materials Chemistry C*, 43432, 2018, 6, 12079-12085

Richard CJ, **Macmillan D**, Hogarth G, Microwave-assisted synthesis of cyclopentadienone iron tricarbonyl complexes: molecular structures of [{h4-C4R2C(O)C4H8}Fe(CO)3] (R = Ph, 2,4-F2C6H3, 4-MeOC6H4) and attempts to prepare Fe(II) hydroxycyclopentadienyl-hydride complexes, *Transition Metal Chemistry*, 2018, **43**, 421-430

Ridley CJ, Daisenberger D, Wilson CW, Stenning GBG, **Sankar G**, Knight KS, Tucker MG, Smith RI, Bull CL, High-Pressure Study of the Elpasolite Perovskite La₂NiMnO₆, *Inorganic Chemistry*, 2019, **58**, 9016-9027

PUBLICATIONS

Robinson MDM, Oropeza FE, Cui M, Zhang KHL, Hohmann MV, Payne DJ, Egdell RG, **Regoutz A**, Electronic Structure of Lanthanide-Doped Bismuth Vanadates: A Systematic Study by X-ray Photoelectron and Optical Spectroscopies, *Journal of Physical Chemistry C*, 2019, **123**, 8484-8499

Rodriguez Arco L, Poma A, Ruiz-Perez L, Scarpa E, Ngamkham K, **Battaglia G**, Molecular bionics – engineering biomaterials at the molecular level using biological principles, *Biomaterials*, 2018, **192**, 26-50

Rogers S, **Catlow CRA**, Gianolio D, Wells PP, Dimitratos N, Supported metal nanoparticles with tailored catalytic properties through sol-immobilisation: applications for the hydrogenation of nitrophenols, *Faraday Discussions*, 2018, **208**, 443-454

Roman M, Dunn A, Taj S, Keolopile ZG, **Rosu-Finsen A**, Gutowski M, McCoustra MRS, Cassidy AM, Field D, Assigning a structural motif using spontaneous molecular dipole orientation in thin films, *Physical Chemistry Chemical Physics*, 2018, **20**, 29038-29044

Rosu-Finsen A, **Salzmann CG**, Origin of the low-temperature endotherm of acid-doped ice VI: new hydrogen-ordered phase of ice or deep glassy states?, *Chemical Science*, 2019, **10**, 515-523

Ruiz-Pérez L, Hurley C, Tomás S, **Battaglia G**, Separating extreme pH gradients using amphiphilic copolymer membranes, *ChemPhysChem*, 2018, **19**, 1987-1989

Rzepa HS, Arkhipenko S, Wan E, Sabatini MT, Karaluka V, Whiting A, **Sheppard TD**, An Accessible Method for DFT Calculation of ¹¹B NMR Shifts of Organoboron Compounds, *Journal of Organic Chemistry*, 2018, **83**, 8020-8025

Sabatini M, Boulton LT, Sneddon HF, **Sheppard TD**, A green chemistry perspective on catalytic amide bond formation, *Nature Catalysis*, 2019, **2**, 43009

Sachs M, Park JS, Pastor E, Kafizas A, Wilson AA, Francàs L, Gul S, Ling M, **Blackman C**, Yano J, Walsh A, Durrant JR, Effect of oxygen deficiency on the excited state kinetics of WO₃ and implications for photocatalysis, *Chemical Science*, 2019, **10**, 5667-5677

Sachs M, Sprick RS, Pearce D, Hillman S, Monti A, Guilbert A, Nick B, Dimitrov S, Shi X, Blanc F, **Zwijnenburg MA**, Nelson J, Durrant J, Cooper A, Understanding structure-activity relationships in linear polymer photocatalysts for hydrogen evolution, *Nature Communications*, 2018, **9**, 4968

Sae-Kung C, Wright BF, Clarke TM, Wallace GG, Mozer AJ, Effects of Interfacial Layers on the Open Circuit Voltage of Polymer/Fullerene Bulk Heterojunction Devices Studied by Charge Extraction Techniques, ACS Applied Materials & Interfaces, 2019, 11, 21030-21041

Salzmann CG, Advances in the experimental exploration of water's phase diagram, *Journal of Chemical Physics*, 2019, 150, 060901

Salzmann CG, Sharif Z, Bull CL, Bramwell ST, Rosu-Finsen A, Funnell NP, Ammonium Fluoride as a Hydrogen-Disordering Agent for Ice, *The Journal of Physical Chemistry C*, 2019, **123**, 16486-16492

Samanta S, Bodrenko I, **Acosta-Gutierrez S**, D'Agostino T, Pathania M, Ghai I, Schleberger C, Bumann D, Wagner R, Winterhalter M, Van Den Berg B, Ceccarelli M, Getting drugs through small pores: Exploiting the porins pathway in Pseudomonas aeruginosa, *ACS Infectious Diseases*, 2018, **4**, 1519-1528

Sandhu A, Walker O, Nistal A, Choy K, **Clancy A**, Perfluoroalkane wax infused gels for effective, regenerating, anti-icing surfaces, *Chemical Communications*, 2019, 55, 3215-3218

Sanz-Sanz C, **Worth GA**, Field modified spin—orbit potential curves of IBr. Preliminary dynamical results, *Physical Chemistry Chemical Physics*, 2019, **21**, 14429-14439

Sari WP, **Blackman C**, Zhu Y, Covington J, AACVD Grown WO₃ Nanoneedles Decorated with Ag/Ag₂O Nanoparticles for Oxygen Measurement in a Humid Environment, *IEEE Sensors Journal*, 2018, **19**, 826-832

Savory CN, **Scanlon DO**, The complex defect chemistry of antimony selenide, *Journal of Materials Chemistry A*, 2019, **7**, 10739-10744

Seavill P, Holt KB, Wilden JD, Electrochemical Preparation and Applications of Copper(I) Acetylides: A Demonstration of How Electrochemistry Can Be Used to Facilitate Sustainability in Homogeneous Catalysis, *Green* Chemistry, 2018, 20, 5474-5478 Selim S, Francàs L, García-Tecedor M, Corby S, **Blackman C**, Gimenez S, Durrant JR, Kafizas A, WO₃/BiVO₄: impact of charge separation at the timescale of water oxidation, *Chemical Science*, 2019, **10**, 2643-2652

Sener ME, **Caruana DJ**, Modulation of Copper(I) oxide reduction/oxidation in Atmospheric Pressure Plasma Jet, *Electrochemistry Communications*, 2018, **95**, 38-42

Shaikh J, Freeman DME, Bronstein H, Clarke TM, Energy-Transfer Pathways and Triplet Lifetime Manipulation in a Zinc Porphyrin/F8BT Hybrid Polymer, *Journal of Physical Chemistry C*, 2018, 122, 23950-23958

Shamsabadi A, **Chudasama V**, A facile route to 1H- and 2H-indazoles from readily accessible acyl hydrazides by exploiting a novel aryne-based molecular rearrangement, *Chemical Communications*, 2018, **54**, 11180-11183

Shamsabadi A, **Chudasama V**, Recent advances in metal-free aerobic C-H activation, *Organic & Biomolecular Chemistry*, 2019, **17**, 2865-2872

Sheppard TD, Hailes HC, Benhamou L, Ward D, Bucar D-K, Lye G, Foster R, Tame C, Wheelhouse K, Sloan L, Functionalised tetrahydrofuran fragments from carbohydrates or sugar beet pulp biomass, *Green Chemistry*, 2019, 21, 2035-2042

Silveri F, Quesne MG, Roldan A, De Leeuw NH, **Catlow CRA**, Hydrogen adsorption on transition metal carbides: A DFT study, *Physical Chemistry Chemical Physics*, 2019, **21**, 5335-5343

Sinclair RC, **Coveney PV**, Modeling Nanostructure in Graphene Oxide: Inhomogeneity and the Percolation Threshold, *Journal of Chemical Information and Modeling*, 2019, **59**, 2741-2745

Sinclair RC, Suter JL, **Coveney PV**, Micromechanical exfoliation of graphene on the atomistic scale, *Physical Chemistry Chemical Physics*, 2019, **21**, 5716-5722

Slater B, Michaelides A, Surface premelting of water ice, *Nature Reviews Chemistry*, 2019-03, 2019, **3**, 172-188

Slater B, Wong SO, Duckworth A, White AJP, Hill MR, Ladewig BP, Upcycling a plastic cup: One-pot synthesis of lactate containing metal organic frameworks from polylactic acid, *Chemical Communications*, 2019, **55**, 7319-7322

Smelt CLC, Sanders VR, Newcombe J, Burt RP, **Sheppard TD**, Topf M, Millar NS, Identification by virtual screening and functional characterisation of novel positive and negative allosteric modulators of the α7 nicotinic acetylcholine receptor, *Neuropharmacology*, 2018, **139**, 194-204

Smith RL, Vickers M, Rosillo-Lopez M, **Salzmann CG**, Stacking Disorder by Design: Factors Governing the Polytypism of Silver lodide upon Precipitation and Formation from the Superionic Phase, *Crystal Growth and Design*, 2019, **19**, 2131-2138

Song J, Liu Z, Wang X, Liu H, Lu Y, Deng X, **Carmalt CJ**, **Parkin IP**, High-Efficiency Bubbles Transportation in Aqueous Environment on Serial-Wedge-Shaped Wettability Pattern, *Journal of Materials Chemistry A*, 2019, **7**, 13567-13576

Song Y, Mobley JK, Motagamwala AH, **Isaacs M**, Dumesic JA, Ralph J, Lee AF, Wilson K, Crocker M, Gold-catalyzed conversion of lignin to low molecular weight aromatics, *Chemical Science*, 2018, **9**, 8127-8133

Sedov IA, Salikov TM, Wadawadigi A, Zha O, Qian E, Acree WE Jr, and **Abraham MH**, Abraham model correlations for describing the thermodynamic properties of solute transfer into pentyl acetate based on headspace chromatographic and solubility measurements, *J. Chem. Thermodynam*, 2018, 124, 133-140

Sprick RS, Bai Y, Gulbert A, Zbiri M, Aitchison C, Wilbraham L, Dan Y, Woods D, **Zwijnenburg MA**, Cooper A, Photocatalytic Hydrogen Evolution from Water Using Fluorene and Dibenzothiophene Sulfone-Conjugated Microporous and Linear Polymers, *Chemistry of Materials*, 2019, **31**, 305-313

Stepanek P, **Sanchez-Perez C**, Telkki V-V, Zhivonitko VV, Kantola AM, Highthroughput continuous-flow system for SABRE hyperpolarization, *Journal of Magnetic Resonance*, 2019, **300**, 008-17

Succi S, Coveney PV, Big data: The end of the scientific method?, Philosophical Transactions of the Royal Society A: Mathematical, *Physical and Engineering Sciences*, 2019, **377**, 20180145

Sun H, Parlett CMA, **Isaacs MA**, Liu X, Adwek G, Wang J, Shen B, Huang J, Wu C, Development of Ca/KIT-6 adsorbents for high temperature CO2 capture, *Fuel*, 2019, **235**, 1070-1076

Sun J, Cheng W, Song J-L, Lu Y, Sun Y-K, Huang L, Liu X, Jin Z-J, Carmalt CJ, Parkin IP, Fabrication of Superhydrophobic Micro Post Array on Aluminum Substrates Using Mask Electrochemical Machining, *Chinese Journal of Mechanical Engineering*, 2018, **31**, 72

Suter T, Brázdová V, McColl K, Miller TS, Nagashima H, Salvadori E, **Sella A**, Howard CA, Kay CWM, **Corà F**, **McMillan PF**, Synthesis, Structure and Electronic Properties of Graphitic Carbon Nitride Films, *Journal of Physical Chemistry C*, 2018, **122**, 25183-25194

Suter TM, Miller TS, Cockcroft JK, Aliev AE, Wilding MC, Sella A, Cora F, Howard CA, McMillan PF, Formation of an ion-free crystalline carbon nitride and its reversible intercalation with ionic species and molecular water, *Chemical Science*, 2019, 10, 2519-2528

Swallow JEN, Williamson BAD, Birkett M, Abbott A, Farnworth M, Featherstone TJ, Peng N, Cheetham KJ, Warren P, Regoutz A, Duncan DA, Lee T-L, Scanlon DO, Dhanak VR, Veal TD, A hard x-ray photoemission study of transparent conducting fluorine-doped tin dioxide, 2018 IEEE 7th World Conference on Photovoltaic Energy Conversion (WCPEC) (A Joint Conference of 45th IEEE PVSC, 28th PVSEC & 34th EU PVSEC), 2018, 3051-3055

Tajuddin NA, Manayil JC, **Isaacs MA**, Parlett CMA, Lee AF, Wilson K, Alkali-Free Zn-Al Layered Double Hydroxide Catalysts for Triglyceride Transesterification, *Catalysts*, 2018, **8**, 667

Thornton G, Allan M, Grinter D, Dhaliwall S, Muryn C, Forrest T, Maccherozzi F, Dhesi SS, Redox behaviour of a Ceria-Zirconia Inverse Model Catalyst, *Surface Science*, 2019, **682**, 41487

Tian X, Hussain S, de Pace C, Ruiz-Pérez L, **Battaglia G**, ZnII Complexes for Bioimaging and Correlated Applications, *Chemistry - An Asian Journal*, 2019, **14**, 509-526

Tian X, Liu T, Fang B, Wang A, Zhang M, Hussain S, Luo L, Zhang R, Zhang Q, Wu J, **Battaglia G**, Li L, Zhang Z, Tian Y, NeuN-Specific Fluorescent Probe Revealing Neuronal Nuclei Protein and Nuclear Acids Association in Living Neurons under STED Nanoscopy, *ACS Applied Materials & Interfaces*, 2018, **10**, 31959-31964

Tombesi A, Li S, Sathasivam S, Page K, Heale FL, Pettinari C, **Carmalt CJ**, **Parkin IP**, Aerosol-assisted chemical vapour deposition of transparent superhydrophobic film by using mixed functional alkoxysilanes, *Scientific Reports*, 2019, **9**, 7549

Tranter A, Love PJ, Mintert F, **Coveney PV**, A Comparison of the Bravyi-Kitaev and Jordan-Wigner Transformations for the Quantum Simulation of Quantum Chemistry, *Journal of Chemical Theory and Computation*, 2018, **14**, 5617-5630

Trantidou T, **Regoutz A**, Voon XN, Payne DJ, Ces O, A "cleanroom-free" and scalable manufacturing technology for the microfluidic generation of lipid-stabilized droplets and cell-sized multisomes, *Sensors and Actuators B-Chemical*, 2018, **267**, 34-41

Treacy JPW, Hussain H, Torrelles X, Cabailh G, Bikondoa O, Nicklin C, **Thornton G**, Lindsay R, Structure of a Superhydrophilic Surface: Wet Chemically Prepared Rutile-TiO2(110) (1 x 1), *Journal of Physical Chemistry C*, 2019, 123, 8463-8468

Twyman NM, Tetzner K, Anthopoulos TD, Payne DJ, **Regoutz A**, Rapid photonic curing of solution-processed In2O3 layers on flexible substrates, *Applied Surface Science*, 2019, **479**, 974-979

Unwin DG, Ghosh S, Ridley F, Richmond MG, **Holt KB**, Hogarth G, Models of the iron-only hydrogenase enzyme: structure, electrochemistry and catalytic activity of $Fe_2(CO)_3(\mu\text{-dithiolate})(\mu,\kappa^1,\kappa^2\text{-triphos})$, *Dalton Transactions*, 2019, **48**, 6174-6190

Vamvakeros A, Jacques SDM, Di Michiel M, Matras D, Middelkoop V, Ismagilov IZ, Matus EV, Kuznetsov VV, Drnec J, Senecal P, **Beale AM**, 5D operando tomographic diffraction imaging of a catalyst bed, *Nature Communications*, 2018, **9**, 4751

Vassaux M, Richardson RA, Coveney PV, The heterogeneous multiscale method applied to inelastic polymer mechanics, *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 2019, **377**, 20180150

Abraham MH, Elguero J and Alkorta I, The hydrogen-bond basicity of carbenes, *Croat. Chem. Acta*, 2018, 91, 121-124

Vogel A, Forster M, Wilbraham L, Smith C, Cowan A, **Zwijnenburg MA**, Sprick RSS, Cooper A, Photocatalytically Active Ladder Polymers, *Faraday Discussions*, 2019, **215**, 84-97

PUBLICATIONS

Wahila MJ, Lebens-Higgins ZW, Butler KT, Fritsch D, Treharne RE, Palgrave RG, Woicik JC, Morgan BJ, Walsh A, Piper LFJ, Accelerated optimization of transparent, amorphous zinc-tin-oxide thin films for optoelectronic applications, APL Materials, 2019, 7, 022509

Walsh A, Scanlon DO, Wei SH, Preface for Special Topic: Earth abundant materials in solar cells, APL Materials, 2018, 6, 84401

Walsh A, Sokol AA, Buckeridge J, Scanlon DO, Catlow CRA, Oxidations States and Ionicity, Nature Materials, 2018, 17, 958-964

Wang X, Chen L, Chong SY, Little MA, Wu Y, Zhu W-H, Clowes R, Yan Y, Sprick RS, Zwijnenburg MA, Cooper AI, Sulfone-containing covalent organic frameworks for photocatalytic hydrogen evolution from water, Nature Chemistry, 2018, 10, 1180-1189

Wang X, Lu Y, Carmalt CJ, Parkin IP, Zhang X, Multifunctional Porous and Magnetic Silicone with High Elasticity, Durability, and Oil-Water Separation Properties, Langmuir, 2018, 34, 13305-

Wang Y, Silveri F, Bayazit MK, Ruan Q, Li Y, Xie J, Catlow CRA, Tang J, Bandgap Engineering of Organic Semiconductors for Highly Efficient Photocatalytic Water Splitting, Advanced Energy Materials, 2018, 8, 1801084

Wang Z, Ganose AM, Niu C, Scanlon DO, Two-dimensional eclipsed arrangement hybrid perovskites for tunable energy level alignments and photovoltaics, Journal of Materials Chemistry C, 2019, **7**, 5139-5147

Wang Z, Roffey A, Losantos R, Lennartson A, Jevric M, Petersen AU, Quant M, Dreos A, Wen X, Sampedro D, Börjesson K, Moth-Poulsen K, Macroscopic heat release in a molecular solar thermal energy storage system, Energy and Environmental Science, 2019, **12**, 187-193

Warne EM, Downes-Ward B, Woodhouse J, Parkes MA, Bellshaw D, Springate E, Majchrzak P, Zhang Y, Karras G, Wyatt AS, Chapman RT, Kirrander A, Minns RS, Photodissociation dynamics of CH_aI probed via multiphoton ionisation photoelectron spectroscopy, Physical Chemistry Chemical Physics, 2019, 21, 11142-11149

Wheatley AM, Kaduk JA, Vickers M, Gindhart AM, Sunzeri JG, Blanton TN, Crystal structure of terazosin hydrochloride dihydrate (Hytrin®), $C_{19}H_{26}N_5O_4CI(H_2O)_2$, Powder Diffraction, 2018, 33, 229-236

Whitehouse WL, Noble JE, Ryadnov MG, Howorka S. Cholesterol Anchors Enable Efficient Binding and Intracellular Uptake of DNA Nanostructures, Bioconjugate Chemistry, 2019, 30, 1836-1844

Wilbraham L, Sprick S, Jelfs K, Zwijnenburg M, Mapping Binary Copolymer Property Space with Neural Networks, Chemical Science, 2019, 10, 4973-4984

Williamson BAD, Buckeridge J, Chadwick NP, Sathasivam S, Carmalt CJ, Parkin IP, Scanlon DO, Dispelling the Myth of Passivated Codoping in TiO2, Chemistry of Materials, 2019, 31, 2577-2589

Wolf M, Gibson EK, Olivier EJ, Neethling JH, Catlow CRA, Fischer N, Claevs M, Water-Induced Formation of Cobalt-Support Compounds under Simulated High Conversion Fischer-Tropsch Environment, ACS Catalysis, 2019, 9, 4902-4918

Wolf M, Gibson EK, Olivier EJ, Neethling JH, Catlow CRA, Fischer N, Claeys M, In-depth characterisation of metal-support compounds in spent Co/SiO₂ Fischer-Tropsch model catalysts, Catalysis Today, 2019, 374, 199-207

Woodhouse JL, Henley A, Parkes MA, Fielding HH, Photoelectron Imaging and Quantum Chemistry Study of Phenolate, Difluorophenolate and Dimethoxyphenolate Anions, Journal of Physical Chemistry A, 2019, 123, 2709-2718

Woodley SM, Lazauskas T, Illingworth M, Carter AC, Sokol AA, What is the best or most relevant global minimum for nanoclusters? Predicting, comparing and recycling cluster structures with WASP@N, Faraday Discussions, 2018, **211**, 593-611

Wright D, Richardson R, Coveney PV, Practical challenges for biomedical modeling using HPC, PeerJ Preprints, 2018, 6, e27299v1

Wright DW, Wan S, Meyer C, van Vlijmen H, Tresadern G, Coveney PV, Application of ESMACS binding free energy protocols to diverse datasets: Bromodomain-containing protein 4, Scientific Reports, 2019, 9, 6017

Wu K, Douglas SP, Wu G, MacRobert AJ, Allan E, **Knapp CE**, **Parkin IP**, A rugged, self-sterilizing antimicrobial copper coating on ultra-high molecular weight polyethylene: A preliminary study on the feasibility of an antimicrobial prosthetic joint material, Journal of Materials Chemistry B, 2019, 7, 3310-3318

Xi F, Bogdanoff P, Harbauer K, Plate P, Höhn C, Rappich J, Wang B, Han X, van de Krol R, Fiechter S, Structural Transformation Identification of Sputtered Amorphous MoSx as an Efficient Hydrogen-Evolving Catalyst during Electrochemical Activation, ACS Catalysis, 2019, 9, 2368-2380

Xia X, Taylor A, Zhao Y, Guldin S, Blackman CS, Use of a New Non-Pyrophoric Liquid Aluminum Precursor for Atomic Layer Deposition, Materials, 2019, 12, 1429

Xie J, Jin R, Li A, Bi Y, Ruan Q, Deng Y, Zhang Y, Yao S, Sankar G, Ma D, Tang J, Highly selective oxidation of methane to methanol at ambient conditions by titanium dioxide-supported iron species, Nature Catalysis, 2018, 1, 889-896

Xu H, Han X, Li Z, Liu W, Li X, Wu J, Guo Z, Liu H, Epitaxial Growth of Few-Layer Black Phosphorene Quantum Dots on Si Substrates, Advanced Materials Interfaces, 2018, 5, 1801048

Xu S, Xu Y, Zhao H, Xu R, Lei Y, Sensitive Gas-Sensing by Creating Adsorption Active Sites: Coating an SnO Layer on Triangle Arrays, ACS Applied Materials & Interfaces, 2018, 10, 29092-29099

Xu Y, Bahmani F, Zhou M, Li Y, Zhang C, Liang F, Kazemi SH, Kaiser U, Meng G, Lei Y, Enhancing potassium-ion battery performance by defect and interlayer engineering, Nanoscale Horizons, 2019, 4, 202-207

Xu Y, Bauer D, Lübke M, Ashton TE, Zong Y, Darr JA, High-power sodium titanate anodes; a comparison of lithium vs sodium-ion batteries, Journal of Power Sources, 2018, 408, 28-37

Xu Y, Dong H, Zhou M, Zhang C, Wu Y, Li W, Dong Y, Lei Y, Ammonium Vanadium Bronze as a Potassium-Ion Battery Cathode with High Rate Capability and Cyclability. Small Methods, 2018, 3, 1800349

Yan R, Yalinca H, Paoletti F, Gobbo F, Marchetti L, Kuzmanic A, Lamba D, Gervasio FL, Konarev PV, Cattaneo A, Pastore A. The Structure of the Prodomain of Mouse proNGF in Contact with the NGF Domain, Structure, 2019, **27**, 78-89

Yeandel SR, Scanlon DO, Goddard P, Enhanced Li-ion dynamics in trivalently doped lithium phosphidosilicate Li2SiP2: a candidate material as a solid Li electrolyte, Journal of Materials Chemistry A, 2019, 7, 3953-3961

Acree WE Jr, and **Abraham MH**, Comment on "Thermodynamic modelling for solubility of 3-methyl-2-nitrobenzoic acid in nine organic solvents from T(283.15-318.15 K) and dissolution properties", *J. Solution Chem.*, 2019, **48**, 163-168

Yim CM, Chen J, Zhang Y, Shaw B-J, Pang CL, Grinter DC, Bluhm H, Salmeron M, Muryn CA, Michaelides A, **Thornton G**, Visualization of Water-Induced Surface Segregation of Polarons on Rutile TiO2(110), *Journal of Physical Chemistry Letters*, 2018, **9**, 4865-4871

Zachariou A, Hawkins A, Lennon D, Parker SF, Suwardiyanto, Matam SK, **Catlow CRA**, Collier P, Hameed A, McGregor J, Howe RF, Investigation of ZSM-5 catalysts for dimethylether conversion using inelastic neutron scattering, *Applied Catalysis A: General*, 2019, **569**, 001-7

Zakaria SNA, Hollingsworth N, Islam HU, Roffey A, Santos-Carballal D, Roldan A, Bras W, Sankar G, Hogarth G, Holt KB, de Leeuw NH, Insight into the Nature of Iron Sulfide Surfaces During the Electrochemical Hydrogen Evolution and CO2 Reduction Reactions, *ACS Applied Materials & Interfaces*, 2018, 10, 32078-32085

Zanetti-Domingues LC, Korovesis D, Needham SR, Tynan CJ, Sagawa S, Roberts SK, Kuzmanic A, Ortiz-Zapater E, Jain P, Roovers RC, Lajevardipour A, van Bergen En Henegouwen PMP, Santis G, Clayton AHA, Clarke DT, **Gervasio FL**, Shan Y, Shaw DE, Rolfe DJ, Parker PJ, Martin-Fernandez ML, The architecture of EGFR's basal complexes reveals autoinhibition mechanisms in dimers and oligomers, *Nature Communications*, 2018, **9**, 4325

Zeinalipour-Yazdi CD, Hargreaves JSJ, Laassiri S, **Catlow CRA**, The integration of experiment and computational modelling in heterogeneously catalysed ammonia synthesis over metal nitrides, *Physical Chemistry Chemical Physics*, 2018, **20**, 21803-21808

Zhang M, Garcia-Araez N, Hector AL, Owen JR, **Palgrave RG**, Palmer MG, Soule S, Solvothermal water-diethylene glycol synthesis of LiCoPO4 and effects of surface treatments on lithium battery performance, *RSC Advances*, 2019, **9**, 740-752

Zhang X, Rabee AIM, **Isaacs M**, Lee AF, Wilson K, Sulfated Zirconia Catalysts for D-Sorbitol Cascade Cyclodehydration to Isosorbide: Impact of Zirconia Phase, *ACS Sustainable Chemistry and Engineering*, 2018, **6**, 14704-14712

Zhao J, Méndez-Sánchez D, Ward JM, Hailes HC, Biomimetic Phosphate-Catalyzed Pictet-Spengler Reaction for the Synthesis of 1,1'-Disubstituted and Spiro-Tetrahydroisoquinoline Alkaloids, *Journal of Organic Chemistry*, 2019, **84**, 7702-7710

Zhu J, Chen J, Xu H, Sun S, **Xu Y**, Zhou M, Gao X, Sun Z, Plasma-Introduced Oxygen Defects Confined in Li4Ti5O12 Nanosheets for Boosting Lithium-Ion Diffusion, *ACS Applied Materials & Interfaces*, 2019, **11**, 17384-17392

Zhu X, Gupta K, Bersani M, **Darr JA**, Shearing PR, Brett DJL, Electrochemical reduction of carbon dioxide on copperbased nanocatalysts using the rotating ring-disc electrode, *Electrochimica Acta*, 2018, **283**, 1037-1044

Zhu Y, Poma A, Rizzello L, Gouveia VM, Ruiz-Perez L, **Battaglia G**, Williams CK, Metabolically Active, Fully Hydrolysable Polymersomes, *Angewandte Chemie - International Edition English*, 2019, **58**, 4581-4586

Zhu Y, Zhang M, Luo L, Gill MR, De Pace C, **Battaglia G**, Zhang Q, Zhou H, Wu J, Tian Y, Tian X, NF-κB hijacking theranostic Pt(II) complex in cancer therapy, *Theranostics*, 2019, **9**, 2158-2166

Zou R, Xu M, He SA, Han X, Lin R, Cui Z, He G, Brett DJL, Guo ZX, Hu J, **Parkin IP**, Cobalt nickel nitride coated by a thin carbon layer anchoring on nitrogen-doped carbon nanotube anodes for high-performance lithium-ion batteries, *Journal of Materials Chemistry A*, 2018, **6**, 19853-19862
Zuilhof H, Albada B, Armitage B, **Howorka S**, Nucleic Acids Nanoscience at Interfaces Special Issue, *Langmuir*, 2018, **34**, 14691

Garciadiego Ortega E, **Evans JRG**, On the energy required to maintain an ocean mirror using the reflectance of foam, *Proc. Inst. Mech. Eng. M: J. Engng Maritime Env.* 2019, 233, 388-397

Abraham MH and Acree WE Jr, Descriptors for the α,ω-dicarboxylic acids from oxalic acid to sebacic acid, *Fluid Phase Equilib.*, 2018,416, 11-24

Acree WE Jr, Jodray M and **Abraham MH**, Illustration of the calculation of solute descriptors for maltol from published solubility data, *Phys. Chem. Liquids*, 2018, 56, 403-409

Hart E, Lee G, Qian E, Jodray M, Barrera M, Fisher R, Che M, Liu Y, Zha O, Woods D, Acree WE Jr, and **Abraham MH**, Determination of Abraham model solute descriptors for 4-*tert*-butylbenzoic acid from experimental solubility data in organic mono-solvents, *Phys. Chem. Liquids*, 2019, 57, 445-432

Books

Peter Day, Scientific Tourism: Scientific Tourism: Some places on the way, 2019 (on Kindle & paperback)

C. R. Ganellin, J.-C. Schwartz and H. Stark. Discovery of Pitolisant, the First Marketed Histamine H3-Receptor Inverse Agonist/Antagonist for Treating Narcolepsy. *Successful Drug Discovery*, Vol. 3 (Eds. J. Fischer, C. Klein, W. E. Childers), Wiley-VCH Verlag GmbH&Co. KGaA, Weinheim, Germany, 2018, pp. 359-381.

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