UCL Chemistry **NEWSLETTER**

Contents

Introduction

Many thanks go to Nicola Best for organising this year's newsletter and to Tracy Hankey at UCL Creative Media Services 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.

Welcome to the Newsletter

We are delighted with the results from the 2014 REF exercise for the UCL Chemistry Department. The department was ranked 2nd in the UK (out of 37 departments) for the world-class impact of its research. It was rated 3rd on research power (behind Oxford and Cambridge). We had the third highest number of staff submitted to the REF of any chemistry department and included all academic staff members. What was particularly pleasing of the 248 research papers we submitted, all bar 14 were judged as either world leading or internationally excellent. This is a remarkable achievement and shows the strength of the department in all areas of Organic, Inorganic, Materials, Physical and Computational Chemistry. It was further also pleasing to note that we finished 3rd overall based on grade point average multiplied by number of academic staff as this metric will be used to determine relative funding. The Chemistry Department had the sixth highest grade point average at UCL (up from 23rd in the previous assessment). It was also interesting to learn that we are the highest rated chemistry department in London based on the REF return; this has been looked at closely in South Kensington.

This year Professor Nora de Leeuw left the department to take up the position of Pro Vice Chancellor at Cardiff University. Nora held various roles in the department including Deputy Head Research. One of her many achievements at UCL included the setting up, obtaining funding for and running of the EPSRC engineering doctorate centre M3S. This program will graduate over 100 Eng.D. students.

Dr Simon Banks left the department to take up the role of Faculty Tutor in the Faculty of Engineering Sciences at UCL. Simon was heavily involved with the undergraduates in the department as Departmental Tutor and Deputy Head (Teaching). After 20 years at UCL, Professor Nik Kaltsoyannis will leave in September to take up a position as Head of Computational Chemistry at Manchester University. Nik established computational chemistry of the actinide elements at UCL. He is also known to bowl the odd over of medium pace seamers and the occasional classic straight drive.

This year we welcome Dr Vijay Chudasama; a new appointment as Lecturer in Organic Chemistry. We also welcome Dr Joe Bear and Dr Caroline Knapp as new Ramsay Fellows.

The department has been successful in a wide range of grant applications. One highlight is a grant to Professor Beppe Battaglia from EPSRC for a new Transmission Electron Microscope (£2.5M) which will be able to study samples in liquid flow. This will be the first instrument of its type in the world.

Four staff have been awarded prizes and medals from learned societies; Professor Sally Price was awarded the interdisciplinary award from RSC; Dr David Scanlon the Harrison-Meldola medal from RSC; Professor Geoff Thornton the Tabor medal and prize of the IOP and myself the Griffith medal and prize from IOM3.

The department is currently working on its Athena Swan silver award application for submission in late 2015. Many thanks to the Athena Swan team for all of its work, especially Professor Helen Fielding who is leading the bid.

I wish you all a successful and healthy 2015-16

Yours sincerely

Professor Ivan Parkin

NEW APPOINTMENTS

Academic appointment

Vijay Chudasama

Lecturer

Vijay joined the Chemistry Department as a Lecturer in Organic Chemistry and Chemical Biology in April 2015. He graduated from UCL with an MSci degree in Chemistry (2008) with the Faculty of Mathematical and Physical Sciences Medal. The main highlight of his undergraduate studies was in a project with Dr Jon Wilden on the versatile synthesis of 2,4-substituted oxazoles, for which he and Jon secured the Science, Engineering and Technology (SET) Chemistry award. On a UCL Graduate School Research Scholarship, Vijay obtained his PhD (2011) under the supervision of Prof. Caddick and Dr Fitzmaurice on aerobic C-H activation methodologies. After a year away, he came back to UCL to do his post-doctoral studies with Prof. Caddick and Dr Smith on novel approaches for the modification of proteins. More recently, Vijay was awarded a Ramsay Fellowship and co-founded biologics company, ThioLogics™ (www.thiologics.com), of which he is the Technical Director.

Vijay's current research interests lie in the development and application of novel methodologies in Chemical Biology and Organic Synthesis. He is particularly interested in trying to answer important biological questions through the application of Organic Chemistry. His group tries to do this by designing and tuning a variety of chemical tools (from chemoselective reagents with orthogonal "click" handles to photoswitchable azobenzenes) for the particular system they are studying.

He has really enjoyed the first few months of his lectureship, especially working with the first few people in his team (Max, Joao, Eifion and Antoine). He has also been very fortunate to publish a couple of articles early in his career (feel free to have a look here: http://chudasama-group.eu/publications/) and greatly appreciates all the support he has received.

RETIREMENTS

Mike Williams

Glassblower

Retired on 31st August 2015

Mike joined the department in 1965 when he was 27 years old. The workshop was in the basement, and four moves and 50 years later the workshop has been moved to the first floor! Mike was in charge for 17 years, during this time there have been five glassblowers in whole of UCL. In 1996 Mike took early retirement, but decided to stay on for 3 days a week. After the death of John Hughes in 2005, Mike worked alone until John Cowley joined about five years ago. Unfortunately due to ill heath, Mike is now retiring. Here is what Mike had to say

"Unfortunately due to ill health I am now retiring, I will miss the College but I am sure my wife will keep me busy!

Best wishes to everyone, and don`t work too hard!!

Mike Williams"

Ian Watts

Safety Officer

Retired on 31st August 2015

Ian originally joined UCL in 2001 as the Lab Manager of the Davy Faraday Research Laboratory (DFRL). In 2006 the DFRL moved to the KLB due to RI refurbishment. The move was supposed to be temporary but became permanent and in 2007 the DFRL became members of staff at UCL.

In 2009 Ian became Teaching Lab Manager and in 2012 he went on to become the Safety Officer in Chemistry.

We wish him all the best with his early retirement.

STAFF HIGHLIGHTS AND NEWS

PROMOTIONS

Promoted to Professor

Dr Erik Arstad

Professor in Radiochemistry

Research areas of interest include:

- Design of small molecule radiotracers
- Labelling/Bioconjugation chemistry
- Methods for imaging and tracer evaluation
- Use of tracers to study brain function
- Clinical evaluation of novel tracer

Dr Andrew Beale

Professor of Inorganic Chemistry

Research areas of interest include:

- Solid state chemistry
- Catalytic materials
- Imaging
- Operando
- Structure-Activity

Promoted to Reader

Dr Matthew Powner

Research areas of interest:

- Origins of Life
- Multicomponent reactions
- Nucleotides, peptides and amphiphilies
- Sulfur chemistry
- Phosphorus chemistry
- Photochemistry

Promoted to Senior Lecturer

Dr Chris Blackman

Research areas of interest include:

- Environmental monitoring
- Photocatalysis
- Functionalised nanomaterials
- Atomic layer deposition

Spotlight on Vijay Chudasama

Vijay Chudasama was named by Forbes magazine as one of the world's top scientists under the age of 30.

Chudasama is technical director and co-founder of ThioLogics, a UCL spin out company. ThioLogics develops biotechnology for new drugs, in particular, those that can cleanly and efficiently find their target. This allows, for instance, chemotherapy that only attacks a tumour, and not the healthy tissue that surrounds it. Here we take a look at the man behind ThioLogics.

Tell us about your research:

I have research interests in the development and application of novel methodologies in Chemical Biology and Organic Synthesis. I am particularly interested in creating linkages between cargos (e.g. drugs, fluorophores) and proteins that selectivity bind to certain cells (e.g. antibodies) to allow targeted delivery. My research focuses on creating linkages that are stable and bear orthogonal 'click' handles to allow rapid assembly of multi-functional bioconjugates in a convergent manner.

What it means to have been selected for Forbes 30 under 30:

It's great to be associated with such a talented group of people and Forbes have been great at promoting discussion between those who have been selected.

Faculty teaching award winners announced

We are delighted to announce this year's winners of the Faculty of Mathematical & Physical Sciences Teaching Awards.

These annual awards recognise excellence in teaching by staff and teaching assistants at all levels within the faculty.

The winners were:

Teaching staff:
Dr Helen Grounds (Chemistry)

Postgraduate Teaching Assistant:
Mr Sam Livingstone (Statistical Science)

Support staff:
Mr Bernard Bristoll (Physics & Astronomy)

The department is thrilled for Helen. Dr Helen Grounds is Lab Manager and Senior Research Associate in the department. She led the development of new lab modules for 3rd year undergraduate students, shifting the focus onto core research skills, and away from the abstruse subdivisions of chemistry. She has also worked to develop online resources for students, including videos and social media related to the courses.

She says: "I have been developing laboratory modules for 3rd year chemistry students. In particular one new innovative module brings together traditionally diverse elements of inorganic and organic chemistry to present it as a unified whole to our undergraduates, making connections which while recognised at research level are often not obvious to the undergraduate cohort. The students now learn a much larger range of core research skills compared to a traditional lab course with assessment made against recognised good practice taken from industry and academia. The new course also allows us to accommodate increasing student numbers."

The student nomination for her award praised her "outstanding, professional and remarkably inspiring" contribution to students' education in the department.

Many congratulations to all the winners on delivering a first-class learning experience for our students.

STAFF HIGHLIGHTS AND NEWS

RSC Interdisciplinary Prize

Professor Sally Price was awarded one of the Royal Society of Chemistry's Interdisciplinary Prizes for 2015.

Sally was recognised for her pioneering work at the interface between chemistry and other disciplines.

Sally has been developing computer programs to predict how organic molecules crystallise and the resulting properties. She explains: "These programs test our fundamental understanding of the process of crystallisation and could help with the design of new organic materials with specific properties, such as could be used in new electronic devices, safer explosives or pigments".

Recently, Sally has enjoyed working with scientists in the pharmaceutical industry, testing whether her program calculations can help discover new crystalline forms of drug molecules with the aim of improving the design of pharmaceutical products and their manufacture.

Dr Robert Parker, Chief Executive of the Royal Society of Chemistry said: "It is always a pleasure to recognise excellence in the chemical sciences and I am pleased to acknowledge the illustrious achievements of our prize and award winners this year.

"Whether they work in research, industry or academia, our winners are the very best in their fields, and they can be very proud to follow in the footsteps of some of the most influential and important scientists around the world.

"In a complex and changing world, chemistry and the chemical sciences are vital in responding to some of humanity's biggest challenges and our prize and award winners are at the forefront of meeting that challenge."

Prize winners are evaluated for the originality and impact of their research, as well as the quality of the results which can be shown in publications, patents, or even software. The awards also recognise the importance of teamwork across the chemical sciences, and the abilities of individuals to develop successful collaborations.

Prof Price praised the contribution of her team to the award. She said: "The award is recognising strong interdisciplinary collaborations within UCL, as well as with different universities and industry through the CPOSS project. It started nearly 20 years ago when I formed the essential experimentalist/theory partnership with Prof Derek Tocher (Chemistry), and we expanded into projects with the late Prof Alan Jones (Chemical Engineering), benefitted from computational infrastructure development with Profs Anthony Finklestein and Wolfgang Emmerich (Computer Science) and Prof Richard Catlow. Our current EPSRC project is working with Prof Simon Gaisford in UCL Pharmacy. There are many other staff and students within UCL who are contributing to the interdisciplinary work on controlling and predicting the organic solid state which this prize recognises. Its been great teamwork, which I've really enjoyed."

RSC Harrison-Meldola Memorial Prize

Dr David O Scanlon has been recognised with the Harrison-Meldola Memorial Prize 2015.

David is a Lecturer in Computational, Inorganic and Materials Chemistry in the Department and at Diamond Light Source. The prize recognises his development and application of computational techniques to understanding and predicting the properties of functional semi-conductors for energy applications

He completed a PhD in Chemistry at Trinity College Dublin in 2011 and now leads the Materials Theory Group at UCL. The group comprises three PhD students and three Master students, who use Computational Chemistry techniques to understand and predict the behaviours of solid state materials, primarily for electronic and renewable energy applications.

The group works on understanding the fundamental properties of the materials used in the screens of smart phones, tablets and televisions and the materials used in solar cells, and how these materials can be tweaked to improve performance.

He says: "I am delighted and humbled to accept the Harrison-Meldola Memorial Prize for 2015. This award recognizes work carried out with a myriad of excellent collaborators, in UCL, Diamond Light Source, nationally and internationally, as well as with a host of dedicated and talented students. This prize showcases the importance of predictive modelling of solid state materials and I am excited to watch the future development of this emerging field."

IOM3 Griffith Medal and Prize

The Institute of Materials, Minerals and Mining (IOM3) has awarded this year's Griffith Medal to Prof Ivan Parkin, Head of the Department. Ivan is a mid-career scientist whose whole career has been devoted to the development of new methods to make, characterise and functionally test materials. His work covers solid-state chemistry for bulk materials, thin film coatings through to antimicrobial polymers.

The work is characterised by innovative synthetic insight, the development of new classes of materials and the development of fundamental understanding. His work has already had an immediate commercial, societal and scientific impact. He is cited in the world's top 600 materials scientists, and in the world's top chemists lists based on ESI Thomson analysis. He has more publications in the Journal of Materials Chemistry than any other author.

Well done Ivan!

2014 – 2015 PRIZE WINNERS

We would like to congratulate the following prize winners:

Undergraduate Prize Winners

KATE SANDERS
CK Ingold Prize - For Excellence in Undergraduate Performance

ANDRE SHAMSABADI
CK Ingold Prize - For Excellence in Undergraduate Performance

MATUS DIVEKY
CK Ingold Prize - For Excellence in Undergraduate Performance

JANA OCKOVA
CK Ingold Prize - For Excellence in Undergraduate Performance

RAIF IBRAHIM
CK Ingold Prize - For Excellence in Undergraduate Performance

LOLADE BAMGBELU
CK Ingold Prize - For Excellence in Undergraduate Performance

CIARA PHILLIPS
Neil Sharp Prize - For Excellence in Theoretical (including Computational) Chemistry

JAMES RUSHWORTH
Parke Davis Prize - For Excellence in Medicinal Chemistry

PHILIP REEVES
Harry Poole Prize - For Excellence in Physical Chemistry

HARENA FESSEHAZION
Ronald Nyholm Prize - For Excellence in Inorganic Chemistry

AZIZ KHAN
Charles Vernon Prize - For Excellence in Biological Chemistry

RHYS WILLIAMS
Franz Sondheimer Prize - For Excellence in Organic Chemistry

PhD Prize Winners

This years' **Ramsay Medal Winner is;**
WILLIAM PEVELER for his presentation entitled
`Nanomaterials for Explosives Detection'.

William also won the **Clark Prize** for best PhD presentation in Inorganic Chemistry for this presentation.

NAFSIKA FORTE
Tuffnell Prize (year 2) - For the best student commencing a Ph.D. in the Department of Chemistry, UCL

DOUGAL HOWARD
2013/14 Ronald Gillespie Prize - For the best student in Inorganic/Materials Chemistry proceeding to a Ph.D. at UCL

HA PHONG NGUYEN
2013/14 Badar Prize - For the best student commencing a Ph.D. in Organic Chemistry

HELEN KIMBER
Ewing Prize – For best PhD presentation in Physical Chemistry for her presentation entitled ***"O atom reactivity on interstellar ices"***

ALEXANDER O'MALLEY
Catlow Prize – For best PhD presentation in Computational Chemistry for his presentation entitled ***"Hydrocarbon Dynamics in Zeolites: Computational and Neutron Scattering Studies"***

ANTOINE MARUANI
Davies Prize – For best PhD presentation in Organic Chemistry for his presentation entitled ***"A Novel Class of Tuneable Reagents for Selective Dual Modifications of Proteins"***

DEANS LIST

Congratulations to five Chemistry graduates who have received a commendation for this year's Dean's List.

JOE BARNETT BSc Chemistry

LAURA MARSH MSci Chemistry

PHILIP REEVES MSci Chemistry

KIRSTY SWAMPILLAI MSci Chemistry

RHYS WILLIAMS MSci Chemistry with a European Language

The Dean's List is designed to reward undergraduate students who excel in their chosen field and deserve recognition for their achievements but who may not necessarily receive any other Departmental or Faculty award.

Also, congratulations goes to **ANDRE SHAMSABADI** (MSci Chemistry) for winning this years **Jackson Lewis Scholarship.** The scholarship was founded in 1966 under the will of Mr H. L. Jackson which recognises outstanding academic performance in one year of study.

Well done guys!

2015 ABTA Doctoral Researcher Awards

This year there was strong competition for this award with 156 applications from 49 universities in the UK and the quality was exceptionally high. We are delighted to announce that 1st place for Natural & Life Sciences Category went to our very own Mr Yao Lu (Supervisor: Ivan Parkin, 2nd Supervisor: Claire Carmalt) for his work on 'Designing Robust Self-Cleaning Surfaces' – Many congratulations to him.

The award ceremony started with 2015 DRA Programme Chair, Dr Hasan Yardimci's welcome speech at UCL's Darwin Lecture Theatre on Saturday, 16th of May.

Following the welcome speech, the finalists in the categories of Natural & Life Sciences, Management & Social Sciences, and Engineering Sciences stepped on to the platform to present their research. After the presentations of 15 finalists, there was a break for poster session and reception.

After the break, Professor Denise Lievesley, Dean of Faculty of Social Science and Public Policy, King's College London, gave a speech on Tips for PhD Success and Moving on as a researcher after completing the PhD.

Starting the awards ceremony, Honourable Mentions and Awardees announced in each category. The winners were presented their certificates and awards by Dr Firat Batmaz, Professor Denise Lievesley and Professor Charlie Elliott..

The ceremony ended with closing remarks by Dr. Bilal Gokpinar, ABTA Executive Committee member, and finally the audience gave a standing ovation to all winners and organisers of the 2015 ABTA Doctoral Researcher Awards competition.

Once again we would like to congratulate Yao for his award.

'Thanks to my family and my supervisors Ivan and Claire, and many thanks to the association of British Turkish academics for organizing this event. I greatly enjoy my research and I will carry on working in academia' **by Mr Yao Lu.**

STUDENT HIGHLIGHTS AND NEWS

Chemistry Outreach 2014-15

Dr. Robert Palgrave

For the 2014-15 I took over chairing the Publicity and Recruitment committee from Dr. David Rowley. I'd first like to thank David for his great work over the past years organising the Department's outreach activities.

The Department's outreach programme has a long history, and this year we again ran the ever popular Spectroscopy Day and Adventures in Molecular Science (AIMS) events. On each day over 100 students and teachers came for a taster of University chemistry, lectures, workshops, and a chance to carry out experiments in the Turner Lab. This year Dr. Hugo Bronstein and Dr. Matt Powner spoke at the AIMS event. Hugo gave some great insights into global warming and how we can combat it, while Matt described recent advances uncovering the chemical basis for the origin of life.

In April we welcomed 40 schools for two days of the Salters' Festival in association with the RSC. The Year 7 and 8 students participated in two challenges in the Turner Lab: identification of an unknown chemical using qualitative analysis (which will prepare them well for the new CHEM1101 experiment…), and adjusting concentration to cause a clock reaction to run in exactly one minute. Prizes, sponsored by the RSC, were awarded to the top teams.

We also ran some exciting new events for the first time this year. In association with UCL Widening Participation, we organised the first UCL Chemistry Summer School entitled "Our Material World". Thirty students from under-represented backgrounds attended for a full week of lectures and practicals, culminating with presentations from the students themselves. In the lab students made gold nanoparticles, superconductors and ferrofluids. We also had inspiring lectures from many members of academic staff on a wide range of topics ranging from nanomedicine to interstellar chemistry.

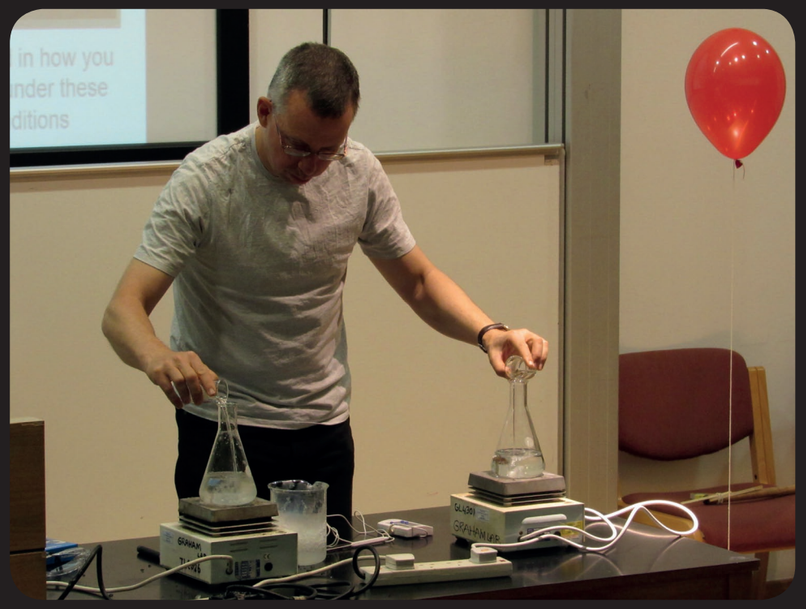
Other events included the "Be a Polymath" event run by one of our alumni Aisha Rahman, and participation in the Natural Science Summer School.

I know many members of academic staff do their own outreach activities. As always I would love to hear about them, and from next year to make this easier there will be a webform available for tracking all departmental outreach activity. This is part of our effort to better understand the impact of our outreach events – by correlating participation by schools in our outreach events with subsequent UCAS application, offers and admissions we can try to measure the effectiveness of what we do.

Next year we have some exciting new developments, including collaborations with two charities. Firstly the RSC will help recruit students for our events and provide funding. We will also work with the Tutorfair Foundation who specialise in providing private tutoring for those who cannot afford it.

None of these activities could run without the dedicated and enthusiastic help of members of staff. I'd like to especially thank the Turner Lab and Graham Lab staff, the many postgraduates who got involved with organisation and running the events, Jamila Yeboah for the administration, the P and R Committee members and of course all the academic staff who have given up their time to be involved.

Chemistry Outreach continued



STUDENT HIGHLIGHTS AND NEWS

Student Conference Reports

By Dr. Laura Fenner

(Research Administration Officer)

This year a number of our postgraduate research students have made use of the Department of Chemistry Student Conference Fund when attending conferences worldwide. A selection of their conference reports are given here.

248th American Chemical Society National Meeting & Exposition
San Francisco, CA, USA
10-14 August 2014

Jarryl D'Oyley 4th year PhD, supervised by Dr. Tom Sheppard

I was fortunate to be accepted to attend the 248th ACS Meeting and Exposition, which took place from 10 – 14th August 2014, in San Francisco. The conference theme was Chemistry and Global Stewardship was intended to provide opportunities for participants to learn more about the latest advances in chemistry.

During the Metal-Mediated Reactions and Syntheses seminar of the Organic Chemistry division on the fourth day of the meeting, I presented my paper entitled Halohydration of alkynols: Au-catalyzed and non-catalyzed routes to α,α-dihalo-β-hydroxyketones. The aim of this oral presentation was to present details of the novel reactions of propargylic alcohols with electrophilic halogen sources with and without gold catalysis, which has been accepted as a journal article by Angewandte Chemie. My presentation was well received; I was asked challenging questions from the audience and was offered suggestions. After the seminar I also discussed the research further with an American PhD student.

The conference had an intense schedule, featuring an impressive line up of plenary speakers presenting their research work over five days. In the organic chemistry sessions, topics covered included studies and developments of metal- and organo-catalysis, syntheses of natural products and a lot of computation and theoretical research. Due to the size of the meeting there were opportunities to attend outside my research field including agrochemistry and environmental chemistry. I feel that these lectures were useful for my awareness of the different applications of organic chemistry.

Although I presented my research on gold-catalysed reactions, the main project of my PhD is the synthesis of small molecules that affect nicotinic receptors. This conference was highly useful for making new contacts and discussions on this topic. This conference is strongly relevant to our work in both areas of research. In summary, this conference has provided me with a wealth of knowledge in the ever growing areas of organic chemistry and medicinal chemistry.

I would like to thank the UCL Chemistry Department for the financial support that allowed me to attend the conference.

Jarryl D'Oyley presenting at the conference.

European Materials Research Society (E-MRS)
Spring Meeting 2015
Lille, France
11-15 May 2015

Neel Makwana 4th year PhD, supervised by Prof. Jawwad Darr

The E-MRS conferences allow information exchange on an interdisciplinary platform, giving delegates the opportunity to discuss technological developments relevant to materials science. The conferences are well attended by a range of scientists from the student to senior level. The Spring meeting provided 32 individual symposia covering a range of topics in 6 categories. My PhD research was directly related to Symposium B, "Materials for applications in water treatment and water splitting", which was also the symposium in which I presented a talk. Attending the conference allowed me to disseminate my research through a formal presentation as well as during networking sessions outside the main conference program. I was able to meet with scientists whose work I am familiar with (through reading publications) and this was an excellent experience; especially when many of these scientists are regarded experts in their field. The discussions that followed my presentation have given me further thoughts relating to the work, which will be discussed in my thesis.

A summary of one conference talk

Title: Exploring the origin of enhanced activity and reaction pathways for photocatalytic hydrogen production on Au/B-TiO2 catalysts

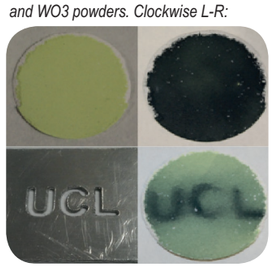
Authors: *Fenglong Wang, Yijiao Jiang, Rose Amal*

Affiliation: School of Chemical Engineering, The University of New South Wales, Sydney, NSW 2052, Australia

In this work, the authors described the hydrogen evolution activity of boron-doped TiO2 and gold-embedded B-TiO2. The catalysts were synthesised by a one-pot sol-gel hydrothermal method. Au/TiO2 showed a higher activity (for hydrogen evolution in a sacrificial system) than bare TiO2 and B-TiO2, whilst Au/B-TiO2 showed the highest photoactivity of all samples. Despite not observing any enhancement in the UV-vis profile for B-TiO2, boron was detected by XPS, and it is thought the presence of Ti−O−B species may contribute to visible light absorption, and hence explain the higher photoactivity achieved. The presence of metal nanoparticles that have a large work function (i.e. a lower Fermi level) can aid electron trapping, which may explain the higher activity shown by the Au/TiO2 sample. With the Au/B-TiO2 sample, the authors suggested that the incorporation of gold ions promoted formation of Ti−O−B species, and upon calcination, the gold ions converted to gold nanoparticles. The combination of Au and Ti−O−B species gave rise to a synergistic effect where the Ti−O−B enhanced light absorption and the Au acted as electron sinks, prolonging charge carrier lifetimes. The authors also demonstrated that H2 could be evolved from pure water, and so conducted studies to determine where the H2 originated from in the sacrificial system. Using isotope labelling it was shown that the majority of H2 originated from the water rather than the methanol used as the sacrificial agent.

Attendance at the conference has developed my ability in presenting scientific information as well as 'thinking outside the box' when responding to questions from other scientists. Whilst our research is a small contribution to the topic area, understanding the work of others helps to put in to perspective how the work relates to the wider community. It was a thoroughly enjoyable and academically stimulating experience.

Figure from Neel Makwana's research showing pressed ceramic wafers of TiO2 and WO3 powders. Clockwise L-R:



(i) WO3 surface of TiO2-WO3 wafer; (ii) discolouration of WO3 surface after shining light on the TiO2 surface; (iii) the appearance of 'UCL' lettering on the WO3 surface after shining light on the TiO2 surface using the template shown in (iv). The discolouration occurs because tungsten in WO3 is reduced to the 5+ oxidation state when electrons (that are photogenerated in TiO2) transfer from TiO2 to WO3.

GABAergic Signalling in Health and Disease: 24th Neuropharmacology Conference 2014
(A Satellite Meeting to Society for Neuroscience)
Sheraton Pentagon City, Arlington, VA, USA
13-14 November 2014

Rosemary Huckvale 4th year PhD, supervised by Dr. Jamie Baker

Summary of conference & experience

This was a two-day satellite meeting to the larger SfN conference, and was designed to bring together researchers to present cutting edge research in this more specific field. Delegates included neurophysiologists as well as pharmacologists and clinicians and so the presented work was varied and showed GABAA receptor research from a number of angles. The research was split into six sections of five talks each: Receptor trafficking and anchoring; Inhibitory synaptogenesis; Chloride homeostasis: Physiology and pathology; Plasticity of GABA receptors; Anesthetics, neurosteroids and ethanol; and Interneurons: co-ordinators of neuronal synchrony. There was also a poster session of around forty posters each day.

Coming from a chemistry background, I was agreeably surprised at the variety as well as the accessibility of the talks, and I really enjoyed presenting my poster to academic staff, post-docs, students and company representatives.

Detailed summary of one conference talk

Regulation of GABAA receptor clustering and trafficking and the tuning of synaptic inhibition1

Professor Josef Kittler, UCL
Though this talk had a general title, it highlighted recent work in his group, which involved the use of an α2-SEP tagged subunit to measure fluorescence of GABAA receptors. α2-SEP fluorescence is pH-dependent and so provides a read-out of the number of receptors on the surface of dendrites and was typically measured at three distinct regions of the cell: the soma, the extrasynaptic regions and at clusters. Decrease in fluorescence indicates receptor internalisation, and this was monitored in live cells during status epilepticus (SE, induced by low Mg2+ treatment). α2-SEP fluorescence at clusters and at extrasynaptic sites decreases, indicating the dispersal of receptors to the soma, where they undergo endocytosis (although the fluorescence at the soma remains steady). Blocking NMDA receptors with an antagonist d-APV blocks this down regulation, which implicates these receptors in this pathway. Concurrent addition of a Ca2+ fluorescent indicator fluo4 shows an increase in intracellular Ca2+ during SE, which is also a sign that NMDA receptors are activated. In fact, when NMDA receptors were activated with NMDA alongside the low Mg2+ treatment, α2-SEP fluorescence in clusters was lost, indicating almost complete dispersal. Calcineurin is a calcium-dependent phosphatase enzyme, and has previously been highlighted as a regulator of GABAergic inhibition. Blocking this enzyme with a peptide during SE inhibited the decrease in surface GABAA receptors, which correlates with the current thoughts that phosphorylation of subunits is thought to cause differences in GABAA receptor mobility, a key part of regulating synaptic inhibition.

It was a good talk to show the power of being able to quantify receptors whilst applying different conditions, and how altering the conditions mean you can pinpoint particular proteins as having importance in a certain signalling pathway. It was also rather nice to see that a lot of work still needs to be done in this area, and ongoing development of new methods and tools, like in my project, are still appreciated. For example, if you were able to track a receptor, you could work out diffusion dynamics under different stimuli.

Benefit of attendance

Firstly, I found it very beneficial to be able to collate my research onto a poster, with practice of writing up results to suit a particular audience (i.e. not a chemistry one). Presenting the poster under the scrutiny of other students as well as academics was both confidence-building and crucial practice for the peer review nature of research in the future. The conference itself was fascinating and I learnt a lot about the importance of interneurons, for example, which are emerging as pivotal regulators of GABAergic inhibition. I also saw research devoted to discovering class-specific therapies for epilepsy, an insight into modern medical research.

[1]Activation of calcineurin underlies altered trafficking of α2 subunit containing $GABA_A$ receptors during prolonged epileptiform activity. Eckel, R., Szulc, B., Walker, M. C., Kittler, J. T.; *Neuropharmacology*, 88 (2015) 82-90.

The Washington Monument.

Nanoparticle Synthesis and Assembly
(Faraday Discussion)
Argonne National Laboratory, Argonne, IL, USA
20-22 April 2015

Anastasia Mantalidi 3rd year PhD, supervised by Prof. Gopinathan Sankar

This conference was an international gathering on the field of nanoparticle synthesis and assembly, and my project is heavily involved with nanoparticle synthesis and characterization. The Faraday Discussion meetings have a unique format where research papers written by the speakers are distributed to all participants before the meeting, and most of the meeting is devoted to discussing the papers while everyone contributes to the discussion - including presenting their own relevant research. The conference was held over the course of two and a half days and the format was exactly that: paper authors gave five minute presentations on their papers and fruitful discussions followed.

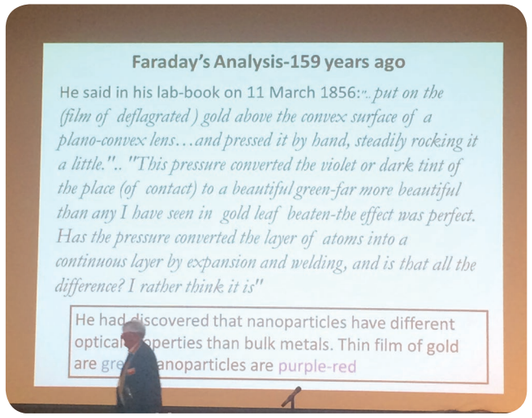
The topics that were covered include magnetism, self-assembly, development of in-situ techniques of monitoring nanoparticle growth and self-assembly, as well as fundamental research on nanoparticle synthesis using solution phase protocols. Scientists and researchers, as well as students from various scientific backgrounds, participated in the very interesting and exciting discussions that took place. The experience of attending such an event is unique because of its format and it constitutes an invaluable learning experience. The fact that the papers are distributed in advance gives the delegates the appropriate time to go over them in detail prior to the meeting, resulting in advanced scientific discussions.

Among other international experts, I had the opportunity to meet Prof. David Schiffrin, one of the two pioneers in the synthesis of thiol-derivatised gold nanoparticles in two – phase liquid method, that is also known as the 'Brust and Schiffrin' method. Additionally, I met Prof. Paul Alivisatos, who is an internationally recognized authority on nanochemistry and a pioneer in the synthesis of semiconductor quantum dots and multi-shaped artificial nanostructures, ranked fifth among the world's 100 top chemists.

An exceptional paper was presented by Dr. Rafal Klajn from the Weizmann Institute of Science, Israel, entitled: Magnetic field-induced self-assembly of iron oxide nanocubes. In their paper, they examine how the shape of the iron oxide nanocrystals affects their self-assembly properties. They evaluated several experimental parameters and they identified the conditions under which the particles can form superstructures including one-dimensional filaments and helices, as well as C-shaped assemblies. These superstructures were reported for the

first time and they have unique properties. Additionally, they performed Monte Carlo simulations to investigate further the mechanisms of self-assembly of these superstructures.

Attending this interactive conference was highly beneficial for my research approach as I was able to keep up with new strategies and trends in nanoscience, and gain knowledge from international experts but also benefit from all the discussions. Additionally, it provided me with the opportunity to demonstrate to an international audience my work by presenting in the lightning presentation session and discussing in my poster session. This international meeting was an ideal meeting to attend because it enhanced my knowledge in the field, in addition to providing an overview of the current state of nanoscience.



Prof. David Schiffrin, in his concluding remarks session, displaying a page from Michael Faraday's lab book showing how enthusiastic he was for research and discovery. Schiffrin mentioned that all young scientists should pursue this enthusiasm in their careers.

2015 Materials Research Society Spring Meeting & Exhibit
San Francisco, CA, USA
6-10 April 2015

Sapna Ponja 2nd year PhD, supervised by Prof. Claire Carmalt

The conference comprised of over 50 technical symposia covering a diverse range of focussed topics in materials chemistry. Two of these were directly relevant to my own research interests: Symposium RR - Solution Syntheses of Inorganic Functional/Multifunctional Materials; and Symposium SS - Oxide Thin Films and Nanostructures for Advanced Electrical, Optical and Magnetic Applications. My poster presentation was given in the RR symposium which included other presentations on thin films of types that I have investigated but using other methods of manufacture (mostly physical vapour deposition). The conference was held in three locations, all easily accessible. The most impressive aspect of the conference was the sheer diversity of symposia and the number of attendees, and of the people I did talk to, most were very enthusiastic about their work and were forthcoming in describing the difficulties that they had to overcome in order to produce their results.

Before attending the conference I had started making films based on silver deposited via aerosol assisted chemical vapour deposition (AACVD). The aim was to manufacture a dielectric/metal/dielectric (DMD) for use as a heat mirror with the silver as the metal in the sandwich. The initial films failed to conduct so it was fortuitous that I was able to attend an oral presentation given by Changho Choi from Oregon State University (USA) titled 'Room temperature highly conductive silver film via a continuous flow microreactor deposition' (Talk RR4.10). Choi described the deposition technique using a modified silver mirror reaction carried out at room temperature without the need of organic precursors. The silver nanocrystalline films had good coverage and reflectance and were as conductive as bulk silver. Choi's future work will consist of making thinner films in order to increase transparency. The standard silver mirror reaction using Tollen's reagent is well-known but modifying it for use in an AACVD application would be a worthwhile challenge in my goal to producing conductive silver films.

The conference was beneficial in a number of ways. First, the poster session that I presented in offered up a number of opportunities to talk to other interested researchers who shared their thoughts and ideas and gave me things to consider in my future experiments. Secondly, I spoke to a number of workers whose focus was on the same metal oxides that I work with which helped to broaden my subject knowledge. Finally, the conference opened my mind to other possible research themes that I could consider post-PhD.

STUDENT HIGHLIGHTS AND NEWS

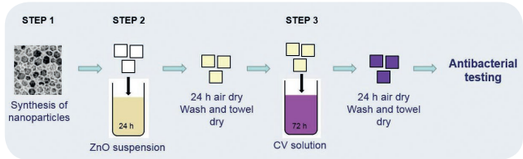
Sandeep Sehmi 2nd year PhD, supervised by Prof. Ivan Parkin

The MRS Spring Meeting was a conference about materials research and it was split between three venues in San Francisco: Marriott Marquis, Moscone West Convention Center and The Park Central Hotel. Registration was on Monday 6th, and the talks were on Tuesday 7th – Friday 10th in the mornings and afternoons. Tuesday, Wednesday and Thursday evenings were allocated to poster presentations, which I attended and also supported other UCL PhD students. My poster session was on Wednesday 8th 8-11pm; around 600 posters were being presented where I had a chance to talk about my work and also look at other projects similar to mine. Some aspects of my work were challenged, mainly because people were not doing similar research to mine and they were unaware of the antibacterial benefits of some of the chemicals and nanoparticles that I use.

It was a very large conference, so every poster session was extremely busy but it meant that a variety of projects were on display at one time. I mainly learnt new ways of synthesising nanoparticles and comparing synthetic methods to the ones I have used myself. I also gained a lot of experience in presenting my work to many people across the world, which I thoroughly enjoyed as other conferences have been smaller and less broad.

I went to talks related to photoactive nanoparticles and nanostructures (Symposium R) because I am interested in synthesising nanoparticles and incorporating them in polymers for antibacterial testing. One talk I went to was given by Alina Chanaewa which was on 'Gold-Zinc Oxide Hybrid Nanosystem for Solar Water Splitting'. It was interesting to me because I have worked with gold and zinc oxide separately and would be interested in combining both to enhance antibacterial activity. She also described that her ZnO nanoparticles were made using oleic acid as a stabilising agent, similar to mine, and I was interested in her results as she used cyclic voltammetry to do so, and I would also like to do this in the future. She found that coupling gold and zinc oxide altered the photocatalytic properties of zinc oxide alone and she was able to create this system using a photocatalytic reaction that yields gold nanoparticle formation exclusively on one side of the ZnO nanoparticles.

This conference was a great opportunity to meet students and researchers as they have given me ideas on how to progress with my research and also it has given me confidence and experience in presenting my work to people who aren't necessarily familiar with my research. I also had an amazing time in San Francisco, particularly because this was the first time I had been there.



Scheme from Sandeep Sehmi's research showing the incorporation of ZnO nanoparticles and crystal violet dye into polyurethane samples for antibacterial testing. Squares indicate the polymer squares used.

The Department of Chemistry Student Conference Fund provides awards of up to £300 per postgraduate research student during their programme of study. Applicants must be presenting a research talk or poster at the conference, and must submit a conference report upon their return in order to receive the award.

To download the regulations and application form please visit the Department of Chemistry Postgraduate Moodle pages.

CHEMISTRY LAB DINNER

Friday 20th November 2015

Due to UCL building works, we have had to make changes to the venue of this year's Chemistry Lab Dinner. The new venue for the dinner will be the Ambassadors Hotel on Upper Woburn Place, only a short walk from the department.

Last years speaker
Prof. Beppe Battaglia

This year's programme will be as follows:-

4.30pm **Nyholm Room**
Meet fellow alumni for tea and coffee

5.00pm **Christopher Ingold Auditorium**
Lecture by Professor Julian Evans

6.00pm **Nyholm Room**
Drinks Reception

7.30pm **Ambassadors Hotel**
12 Upper Woburn Place London, WC1H 0HX
Dinner

10.30pm **Ambassadors Hotel Bar**
For guests that wish to mingle following the dinner, the hotel has a bar area.

The full cost of the evening is £45 for alumni and guests. For current postgraduate students, a limited number of tickets will be charged at £35. This cost includes a 3 course meal with tea and coffee plus half a bottle of wine.

If you wish to attend, please keep an eye out on the Chemistry website for when tickets go on sale, alternatively you can email **n.best@ucl.ac.uk** and Nicola will let you know further details and when tickets are available.

Photos Courtesy of Michael J. Phillips Photography

Obituary

Prof. David P. Craig

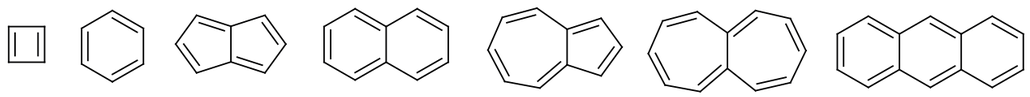
23rd December 1919 – 1st July 2015

We are sad to pass on the news that Prof. David P. Craig FRS FAA died in Canberra on 1 July 2015. David was a Professor of Chemistry at UCL from 1956 to 1967 and then became Foundation Professor of Physical and Theoretical Chemistry at the Research School of Chemistry in the Australian National University, Canberra. Apart from being one of Australia's most accomplished academics and a truly great man, David was instrumental in creating this school and building its national and international reputation. He was a former President of the Australian Academy of Science; David was a gifted lecturer in theoretical chemistry. In his early days he had been a Captain in the Australian Imperial Force against the Japanese from 1941-1944, being based in New Guinea.

David Craig, who was a major figure in theoretical chemistry and in the organisation of Australian education and in science, died at the age of 95 on July 1 in Canberra, Australia. He, with Allan Maccoll and Ron Nyholm, led the influx of Australian research students to the UCL Chemistry Department in the 1940s, 50s, and '60s which so vitalised the department. This article is based heavily on a section of Alwyn Davies and Peter Garratt's book on the History of the Department (UCL Chemistry Department 1828-1974). An extended interview with David is available on the Australian Academy website (https://www.science.org.au/node/327950).

David Craig and Allan Maccoll were together as students at Sydney University. David graduated in 1941. He failed the navy test for colour blindness and did distinguished wartime service as ADC to General Sir Iven Mackay, partly in New Guinea.

In 1944 he joined the staff at Sydney University and in 1946 he followed Allan Maccoll to UCL where he found that "the laboratories were really primitive and dirty, but there was a great spirit". He worked for his Ph.D. on the theory of the excited state of benzene under the nominal supervision of Sir Christopher Ingold, and on graduating, immediately was appointed as a member of staff where he introduced theoretical chemistry to the department. His initial work involved the theoretical interpretation of the spectra and electronic structures and aromatic or antiaromatic character of cyclically conjugated molecules, such as cyclobutadiene, benzene, pentalene, naphthalene, azulene, heptalene, and anthracene which are shown, left to right, in the formulae below. This was done sometimes with people from inside the department such as Allan Maccoll, and Ian Ross, who was one of his first Ph.D. students, and also with outsiders such as Coulson and Pullman. In 1954 he was one of the quintet of Craig, Maccoll, Nyholm, Orgel, and Sutton who published a paper on chemical bonds involving d-orbitals which became a citation classic.



In 1952 David returned to Sydney as the foundation Professor of Physical Chemistry, with Le Fèvre, one of our alumni, as Head of Department and Arthur Birch as organic professor. His stay in Australia was short. "I heard from Ingold that he would like to get me back in his department, having already got Nyholm back from Sydney Technical College. They had everything in equipment and an excellent supply of research students and postdocs - it was irresistible. So I went back in '56". He and his family travelled on the Imperial Star, which took eight passengers. "When we were a day's steaming from Aden the message came through that the Israeli war had broken out, so we did a 90 degree turn to port and went down to Cape Town. It had been a full month from one sight of land to the next, and the crew were pretty restive".

He got interested in the experimental observation of electronic transitions in arenes. "We had a large basement room, D20, chosen to be free of vibrations from the Inner Circle trains and so suitable for a spectroscopy lab. There were larger Hilger spectrographs and a giant grating instrument with high resolution. Ian Ross, who was student of mine, and Gerry King had put up a sign above the door saying "Abandon all hope, ye who enter here"; this was later translated into the original medieval Tuscan, Nevertheless, that was where the spectrum of naphthalene was solved in the grating spectrograph".

To minimise the molecular vibration the spectra had to be recorded at low temperature using liquid hydrogen, and one his students, Peter Hobbins, used to collect this in a Dewar flask from Oxford and bring it back by train. But then the liquid hydrogen plant at Oxford had a huge explosion and David's work had to stop until safe liquid helium became available.

He worked with Edwin Power from the Mathematics Department on dipole-dipole interactions. A number of David's UCL students went on to academic posts in UCL and elsewhere; Stewart Walmsley and Thiru (Thuraiappah Thirunamachandran) were appointed to the UC staff. David and Thiru published together a book on Molecular Quantum Mechanics: An Introduction to Radiation-Molecule Interactions in 1984, republished in 1998, and David and Stuart Walmsley published Excitons in Molecular Crystals.

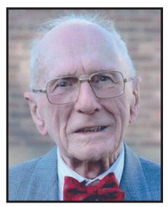
In the middle 1960s the Australian National University in conceived the idea of founding a Research School of Chemistry of a standard that would attract back to Australia the many young chemists who had moved to the UK or USA.

They hoped to recruit Ron Nyholm, Arthur Birch (then at Manchester), and David Craig as the founding professors of inorganic, organic, and physical chemistry respectively, and the three met clandestinely in Brown's Hotel to advise on the design of the department. Ultimately, Ron Nyholm declined the offer but David Craig and Arthur Birch moved to Canberra in 1967. David's experience in helping to plan the Christopher Ingold Laboratory came in valuable in designing the excellent laboratories in Canberra. The Research School of Chemistry became one of international status and did indeed attract back to Australia many of the young chemists who had been at UCL – Martin Bennet, Dick Bramley, Ian Ross, Eric Magnussen, Glen Robertson, Jim Parker, and, in their retirement, Brice Bosnich and Malcolm Gerlock.

David was elected a Fellow of the Royal Society in 1968, and a Fellow of the Australian Academy of Science in 1968. He was Treasurer of the Academy from 1985 to 1989, then President from 1990 to 1994, and made an Officer of the Order of Australia in 1985.

He was an excellent lecturer to undergraduates, supervisor of research students and an able administrator. The Department has lost one of its outstanding post-war alumni.

Obituary



Douglas Ambrose

Died 1st February 2015, aged 95.

Douglas Ambrose, who died in February, was the only member of our pre-war alumni with whom we were in contact. He came to the College in 1936 to do the Intermediate B.Sc,, and graduated with a B.Sc. in Chemistry in 1939. After service in the army during the war, he returned to UCL to work for a Ph.D. with Sir Christopher Ingold. He spent most of his subsequent career at the National Physical Laboratory in Teddington, but when he retired in 1979 he came back on an Honorary appointment, working in the field of thermodynamics in association with Max McGlashan and Mike Ewing.

When we wrote the book on the History of the Department, we appealed to our alumni to send us their memories of their time here, and Douglas sent us a long essay together with photographs taken by his wife, who also was a student in the department. Some excerpts from his essay are reproduced below and paint a very different picture of the College and Department 60 years ago, from that which we know today.

"The Union (for men only) was at the north end of the North Cloisters and the Women's Union (the WUS) was in the South Wing. Each Cloister was provided with a Beadle. Segregation of the sexes extended to the prohibition of personal contact in the Cloisters and one of the duties of the Beadles was to police this. In the summer students could enjoy the sun on the South lawn in the Quad (I think the North was reserved for staff) but they were under the eye of the Tutor to Women Students who had her office in the South wing which overlooked the lawn; propriety was thereby preserved whether she was looking or not. However there was a mixed lounge with bar somewhere in the middle of the College; it was small and often very crowded."

"There were two places where one could eat, the Upper and Lower Refectories. The Upper as was under the Portico. The Lower, which was located down the stairs at the south end of the Cloisters... gave cafeteria service. I usually ate in the Upper which provided waitress service and a three-course meal cost ninepence, two courses only sixpence."

Douglas passed the intermediate examination in chemistry, physics, pure maths and applied maths in 1937 and went on to do a special B.Sc. degree in Chemistry with subsidiary Physics; at that time there was also available an general B.Sc. degree, principally for students who were aiming to be teachers, when they studied three subjects (e.g. Chemistry, Physics, and Biology) at equal standard.

"Those who had taken Inter were now joined by the fresh faces of students who came up already better qualified because they had taken a Higher Certificate or its equivalent in chemistry. We were all due to take our final exams after two years but the University demanded three years of study for the award of a B.Sc. so those who took finals after only two years were then required to spend a further year in postgraduate study. My fees were £49 10s for 1936-37 and £60 18s for each of the two following years."

"In the inorganic lab we started with "spots", identification of inorganic samples, which might have more than one component, by the wet method based on hydrogen sulphide as described in "Qualitative Chemical Analysis " by Alfred A. Noyes. ... The H2S was generated from 3 or 4 Kipps in a walk-in fume room and the atmosphere there was needless to say putrid,.....One of the women students had to be hauled out because she had been overcome. In the next term we moved to quantitative analysis, volumetric and gravimetric, using as a guide "Textbook of Quantitative Analysis" by I.M. Kolthoff and E.B. Sandell".

"The following October we exchanged the stink of H2S for the aroma and teak benches of the organic lab on the floor above. Preparations were done the 10g scale following Julius B Cohen's "Practical Organic Chemistry". No worries about safety; we made benzidine and naphthylamine, and benzene was freely used as a solvent. A feature of the organic lab was the ice store which was a large insulated box somewhere near the middle of the lab. Blocks of ice, perhaps half a hundredweight, were supplied by a firm called Carlo Gatti, who operated all over London The blocks had to be attacked with a hammer and spike to produce large lumps which were fed into a mincer (marketed for the fishing industry) which produced pebble-sized lumps that in turn went into something nearer a domestic scale device to produce crushed ice."

"Practical physical chemistry in the basement came in the summer term when, as with physics, we carried out a prescribed series of experiments but I don't remember much about them".

"In the long vac there was the opportunity of taking a week's course for a charge of £2 2s with Mr Nelson the glass blower and we learnt to join tubing and tried to make a condenser – all in soda glass, and in our beginners' hands the joint usually cracked as it cooled.."

The lecturers:

"Le Fevre wore double-breasted suits and seemed conscious of his dress in contrast to almost all the rest of the staff; in the lectures we somehow always seemed to arrive at Dipole Moments."

"Goodeve was enthusiastic but I am not sure that his "potential function", by which he avoided talking about free energy and entropy, but nobody else used, really helped; we were all made aware that he was a Canadian and an alumnus of Manitoba University and proud of it."

"I think I heard more than once how Brady won the First World War (that is what he seemed to be saying) by solving the problem of the nitration of toluene to get the mixtures of the right melting point."

"Guggenheim, who had written an impenetrable book on thermodynamics, clearly believed that with Willard Gibbs he was the only person to understand the subject,"

"Terry was a lovable person but a terrible lecturer with a smoker's cough but there used to be a rumour that he had been gassed in the war; his lecture notes appeared to be written on the backs of envelopes that he would produce from his jacket usually in the wrong order,"

"Hughes was remarkable in that whenever I met him in later life, he remembered me and also remembered all the others in my year, never mixing them up.

"After the war when I was a research student I found interviews with Ingold difficult because they were punctuated with silences whilst he was thinking, and I would be all the time wondering whether I should say something."

The solution to a problem

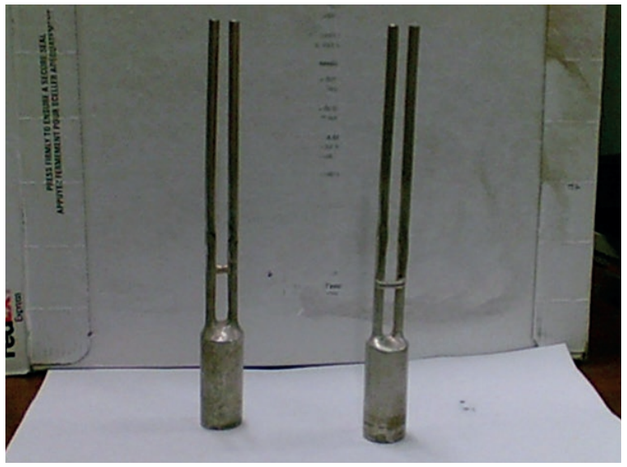
By Professor Alwyn Davies

Last year we found in the departmental safe two silver conical flasks and some unidentified silver devices. We asked through the Newsletter of the RSC Historical Group for help in identifying what they were for. One of our alumni, Dr. Alex Jones, seems to have found the answer in a paper by Edgar Philip Perman in Transactions of the Faraday Society, 1921, **27**, 59-69.

Perman (1866-1947) had been a Cloth Workers Exhibitioner at UCL. In 1889, he published a paper on determining the boiling point of sodium and potassium, thanking William Ramsay for advice. He then appears to have spent all his subsequent career at what is now Cardiff University, working on the physical properties of liquids. His 1921 paper is in part on the vapour pressures of aqueous solutions of sodium hydroxide: he draws air through bubblers containing the solution and estimates the weight of water which evaporates by absorbing it in concentrated sulphuric acid. “The last three (bubblers) were made all in one piece of pure silver, the makers being Walker and Hall, Sheffield. It was essential that they should be made of pure silver to ensure that the solutions should be free of all traces of silicates which would be formed by the action of the strong caustic soda solutions on glass at the high temperatures of the experiments”. He does not show a picture of the bubblers but their capacity of about 30 mL is similar to that of our devices which presumably were intended for some similar purpose.

This identification is strengthened by the fact that he prepared his caustic soda solution in pure silver flasks fitted with a rubber stopper. These could be the equivalent of the silver conical flasks which we found together with the bubblers. The hallmarks on our flasks date them from 1923 but what we now recognise to be the bubblers are not hallmarked.

The question remains as to what these flasks and bubblers, which appear to be unused, were doing in our safe. At the time, F.G. Donnan was Professor of General Chemistry and Norman Collie was Professor of Organic Chemistry, but this silver apparatus does not appear to be immediately relevant to any work which they or their colleagues were publishing.



Calling all Alumni

We would love to hear about your career and life since leaving UCL, with a view to possibly including your story in the next Newsletter.

If you would be willing to write a piece for the next Newsletter, please contact, **Nicola Best** via email:

n.best@ucl.ac.uk with subject heading “Newsletter Alumni”.

Donations

Those UCL Alumni and friends who have supported the department directly help us to build on our international reputation for teaching and research and make a range of exciting activity possible. Your kind contributions have a direct impact upon our students and staff and we are very grateful for it.

Many of the contributions we receive help to fund our awards and student prizes, for example our Ronald Gillespie Award for Inorganic Chemistry and The Viola Horsell legacy is being used to support a number of Impact Scholarships.

We continue to provide an excellent education and training environment for undergraduate and postgraduate students in Chemistry and all of my colleagues 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.

We would like to thank the following UCL Alumni Donors for their help over the last year:-

Dr L Affleck - 2002 PhD [MPhil Chemistry]
Dr D Ambrose, OBE - 1939 Bachelor of Science, 1949 PhD
Dr J H Aupers - 1965 Bachelor of Science
Dr D Baxendale - 1965 PhD
Mr G Belchem - 1993 Bachelor of Science [BSc Chemistry]
Dr A Bradley - 1997 PhD [MPhil Chemistry]
Mr G H Brown - 1953 Bachelor of Science [BSc Chemistry]
Professor Steve Caddick
Mr C Chu - 2011 Master in Science [MSci Chemistry with Mathematics] 2012 Post-Graduate Certificate in Education [PGCE Chemistry]
Squ Leader P Claridge - 1956 Bachelor of Science [BSc Biochemistry]
Professor S Doonan -1962 Bachelor of Science, 1966 PhD
Dr J D Forrester - 1960 PhD [MPhil Chemistry]
Professor P J Garratt
Dr A C Gilby - 1962 PhD [BSc Chemistry]
Miss V Gstettenbauer - 2013 Bachelor of Science [BSc Chemistry]
Mr F W Haslam - 1969 Bachelor of Science
Miss Hedayat-Kelishadi - 2013 Master in Science [MSci Chemistry]
Dr A E Hill
Dr J Michael Hollas - 1956 Bachelor of Science, 1959 PhD
Dr DJ Hulme - 2003 Master in Science [MSci Computer Science with Cognitive Science] 2009 Doctor in Engineering [EngD Virtual Environments Imaging & Visual]
Dr P M Jackson - 1957 Bachelor of Science
Mrs K S Kershaw - 2002 Master in Science [MSci Medicinal Chemistry]
Dr S K Kimpton - 1981 Bachelor of Science [BSc Chemistry], 1984 PhD [MPhil Chemistry]
Dr V J Lees - 2004 Master in Science [MSci Chemistry], 2012 PhD [Research Chemistry]
Dr A J W Lobo - 2007 Master in Science [MSci Chemistry] and 2012 Doctor in Engineering [EngD Molecular Modelling & Materials Simulation]
Dr D J Machin - 1957 Bachelor of Science, 1960 PhD
Dr S C Mangles - 2002 Master in Science [MSci Chemistry], 2006 PhD [Research Chemistry]
Dr D P Mann - 2005 PhD [Research Chemistry]
Professor R V Parish - 1955 Bachelor of Science, 1958 PhD
Dr R Peters - 1977 Bachelor of Science, 1981 PhD
Mrs S P Peters - 1980 Bachelor of Science [BSc Chemistry]
Dr Matthew Edward Popkin - 1998 PhD [MPhil Chemistry]
Mr BJ Merrifield - Master in Science [MSci Chemistry]
Dr A F Richards - 1961 Bachelor of Science, 1964 PhD
Professor E A Robinson - 1955 Bachelor of Science [BSc Chemistry], 1958 PhD [MPhil Chemistry]
Mr N S Rose - 1977 Bachelor of Science [BSc Chemistry]
Dr BK Sharma - 2003 Master in Science [MSci Chemistry], 2010 PhD [Research Chemistry]
Dr A I Sotowicz - 1976 Bachelor of Science [BSc Chemistry]
Mr R H Unthank - 1963 Bachelor of Science [BSc Chemistry]
Dr G Walker
Dr J Wells - 1965 Bachelor of Science [BSc Chemistry]
Dr John Wilby - 1953 Bachelor of Science [BSc Chemistry], 1956 PhD [MPhil Chemistry]

We have made every attempt to ensure the information contained in this list is accurate and up to date. Should you have any queries, please contact **Mr Hamish Stewart** from the Alumni and Relations Department via email at **h.stewart@ucl.ac.uk**

To join your colleagues already enhancing the lives of students and staff in the Chemistry Department please visit the alumni pages on the Chemistry website:
http://www.ucl.ac.uk/chemistry/alumni and follow the ‘give a gift’ link.

You can also download a gift form from at the following link:
http://www.ucl.ac.uk/makeyourmark/how-to-give

The UCL Development & Alumni Relations Office Data Protection statement is available at **http://www.ucl.ac.uk/development/operations/data_protection.**

Please contact us if you would prefer a printed copy.

Materials innovation impact acceleration awards

By Dr. Laura Fenner
(Research Administration Officer)

The Department of Chemistry received a total of six awards in 2014 as part of the internal Materials Innovation Impact Acceleration (MIIA) scheme, which was funded through the EPSRC Impact Acceleration Account (IAA) award made to UCL for 2012-15. The selected projects were expected to lead to impacts outside of academia and the funding was awarded to help with this goal.

In May 2015 all six projects were in the final stages or had already finished, so award holders gathered to present and discuss their progress at the second MIIA update meeting. For each award, a project investigator gave a ten minute presentation which was followed by a discussion with the general audience, and award holders continued to share ideas afterwards over drinks.

Three of the speakers at the meeting report below on their projects, focussing particularly on the impacts that have been achieved.

Application of high performance computing to industrially important metal oxides for catalysis

Dr. Crispin Cooper and Prof. Richard Catlow

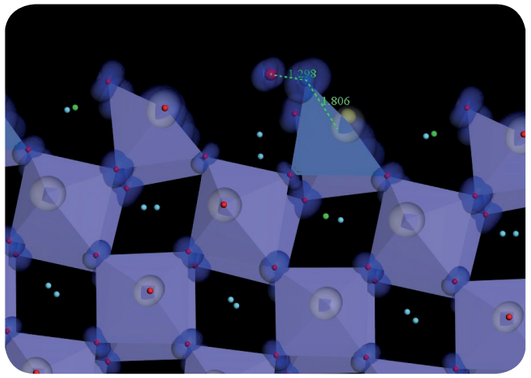
The aim of this MIIA funded project has been to apply high performance computing resources, modelling techniques and knowledge of metal oxide materials in catalysis to explore and understand trends in the catalytic properties of a range of perovskite structure materials. These materials are of great interest to the industrial partner Johnson Matthey due to their potential application in exhaust remediation, particularly their ability to reduce NO_x species as reported in the scientific literature. Perovskite metal oxide materials may be able to replace or reduce the use of costly platinum group metals and enhance the performance of automotive catalysts. There is an existing experimental program being conducted by the industrial partner, which aims to replace platinum group metal based catalysts.

Perovskite structured materials have a basic formula ABO_3, where A is a large and B a smaller metal cation. The particular system of interest is $LaMO_3$ where *M* is a first row transition metal. When A site doping (for example, with Sr^{2+}) is also considered an extremely large range of compositions and structures must be considered. A variety of computational techniques, including rapid screening of thousands of structures with inter-atomic potentials and more detailed electronic structure methods, have been applied in order to improve understanding of this important class of materials. Automated screening has been applied to investigate A site doping, where a 2+ ion is substituted for La^{3+} in the lattice and charge compensated by the creation of oxygen vacancies. The distribution of dopant ions and vacancies in the material allows a huge range of configurations. The relative stability of representative sample configurations and the distribution of energies they cover has been provided by the use of fast inter-atomic potentials modelling and automated sampling.

In order to explore catalytic reactivity, electronic structure (DFT) models have been built, starting with ideal bulk structures and building up to include a large range of compositions, surface configurations and defects, in order to allow important trends to be identified. The interactions of these materials with exhaust gas components have now been modelled for many B site metal ions both with and without A site doping. For example, binding energies for various gas phase species over different surface sites allow significant trends in behaviours as B ions are varied to be explored, while the detailed electronic structure provides understanding of the transfer of electron density between the catalyst surface and substrate molecules. Information from modelling work is of value in guiding the rational design of experimental work, explaining experimental observations and contributes to the development of a detailed mechanistic understanding of catalytic reactions over the perovskite materials. The project has now been continued and brought in house by the industrial partner.

I would like to thank Richard Catlow of UCL Chemistry and Misbah Sarwar at Johnson Matthey for their support during the project.

Crispin Cooper



An image from Dr. Cooper's modelling work of NO binding to a doped perovskite surface site.

RESEARCH HIGHLIGHTS

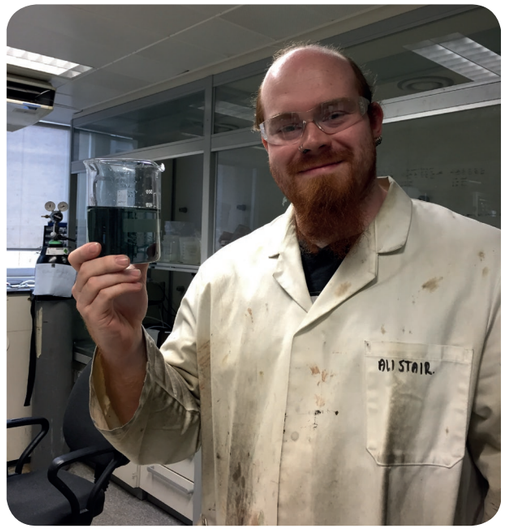
Maximising impact of a new continuous pilot for UK catalysis

Dr. Alistair Holdsworth and Prof. Jawwad Darr

My work as Tech Transfer Research Fellow involves working with a wide range of industrial partners to produce commercially interesting materials using our group's continuous hydrothermal flow synthesis (CHFS) process. I liaise with the scientists in our partner companies to discuss a plan of action, research the best synthetic method and plan the experiments, undertake them and then analyse the produced material before sending it off to them for testing. The overall goal of this process is to move materials up the technology readiness level (TRL) scale in order to move research from academic study to business viability.

I have worked with more than half a dozen industrial partners on a wide range of materials, including pigments, zinc oxide for suncreams, perovskites as dielectrics and charge storage materials, and novel Li-ion battery electrodes. This has involved use of the standard CHFS process and modification of the equipment to allow the production of compounds which would otherwise be difficult to achieve. This has been explored for a range of industrially interesting materials, many of which we are now capable of producing in respectable quantities. This work has resulted in CHFS being utilised for industrial validation, scale up and the manufacture of useful materials on larger scales, thus validating the process as a viable process for industrial production of nanoparticles.

Alistair Holdsworth



Dr. Holdsworth with a suspension of nanoparticles produced using the group's CHFS equipment.

Light activated antimicrobials

Dr. Kristopher Page, Dr. Sacha Noimark and Prof. Ivan Parkin

Hospital acquired infections are estimated to cost the NHS approximately £1,000,000 per annum and 1 in 16 patients pick up an infection whilst in an NHS hospital. In specific clinical situations, such as long term catheterisation, a patient can be almost guaranteed to suffer a medical device related infection. Currently, infections are treated in patients by use of antibiotics, but the over prescription and misuse of these has led to the development of antibiotic resistant bacterial strains. Indeed it has been said that society is heading towards a "post antibiotic era" – one in which previously treatable ailments once again become of serious concern. A shift in strategy towards infection prevention is required – one desirable way to achieve this is to develop antimicrobial surfaces which can remove pathogens from the environment without applying a selective pressure for further development of antimicrobial resistance.

The work funded by the MIIA award has worked to further the ongoing study of light activated antimicrobial (LAA) surfaces within the research group. LAA surfaces are particularly attractive as their antimicrobial function, via radical species generation, has no specific target within a microbe. Their non-specific mode of action means that there is no selective pressure for the expression of antimicrobial resistance.

The main impacts arising from the MIIA award were the ability to generate new classes of antimicrobial surfaces and prototypes and to study types of microorganisms not previously examined in our group.

TiO_2 nanoparticle and Au-TiO_2 nanoparticle encapsulated silicone samples were studied for the first time and the work presented at a Faraday Discussion (FD 175). These materials demonstrated efficacy against both Gram positive and negative bacteria, with an excellent response against S. aureus using a non-light activated mechanism reducing bacterial numbers to below the experimental detection limit [1]. Antimicrobial screen protectors for mobile phones were also developed by utilisation of crystal violet LAA dye. These screen protector foils demonstrated useful efficacy against microbial loads much greater than real word contamination by both Gram positive and negative bacteria [2]. Some commercial interest for this from a technology company was received via UCL Business. In collaboration with Dr. Lena Ciric at UCL Civil Environmental and Geomatic Engineering, we have also been able to study for the first time the action of the LAA surfaces against yeasts (a common catheter related infection organism), bateriophages (an analogue for viruses) and moulds. The LAA samples demonstrated good efficacy against all three of these organisms and a paper is in preparation from this work.

Throughout the work we have developed a number of LAA surfaces and prototype devices, some of which can be seen in **the figure below**. Of particular note, the computer keyboard cover pictured has been tested and used within UCLH and further work to improve the formulation and effectiveness of these prototypes in in progress. There is clearly much work still to do, but we have successfully created a number of prototype items with useful antimicrobial function and with further refinement it is hoped that these might find a use either in a clinical setting or in general use in the near future.

[1] Noimark, S., et al., *FD175: Functionalised Gold and Titania Nanoparticles and Surfaces For Use as Antimicrobial Coatings.* Faraday Discussions, 2014.

[2] Page, K., et al., *Light-activated antibacterial screen protectors for mobile telephones and tablet computers.* Journal of Photochemistry and Photobiology A: Chemistry, 2015. **296**(0): p. 19-24.

Kris Page

A selection of light activated antimicrobial treated products and surfaces. Clockwise from top left: UCLH computer keyboard cover, mobile phone case, mobile phone screen protector, urinary catheters, painted plastic and UCLH computer mouse cover.

The other three awards received by researchers in the Department of Chemistry were:

Graphic carbon nitrides for energy applications –
Dr. Tom Miller, Dr. Furio Cora, Prof. Paul McMillan, Dr. Dan Brett and Dr. Paul Shearing

Novel synthesis method and production of millimetre-sized carbon dioxide capture (and hydrogen purification) –
Prof. Xiao Guo

Integrating nanomaterial formulations into drug discovery –
Prof. Giuseppe Battaglia

New Frontiers in Transition Metal Free Synthesis

Dr Jon Wilden

For many years chemists have been using chemical reactions to build complex molecules for an array of diverse applications. In particular, reactions that create new carbon-carbon and carbon-heteroatom bonds have been particularly powerful and scientists have commonly used catalysts based on transition metals including palladium, nickel, rhodium, ruthenium and platinum to achieve this. Over the last half-century, these mediators and an understanding of their reactivity has led to a revolution in the speed and efficiency that organic molecules can be constructed.

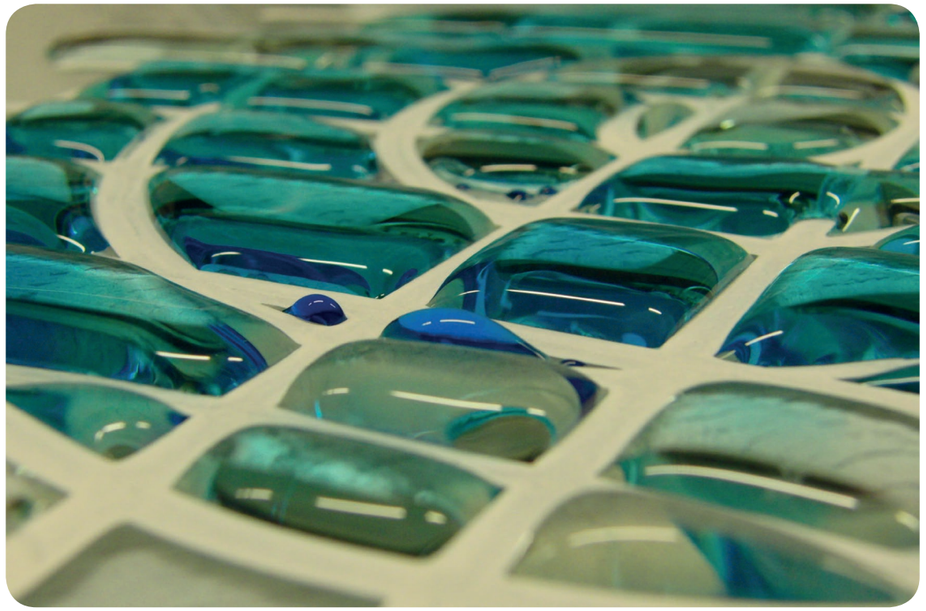
Despite the power of transition metal mediated processes, they are not without their problems, particularly when used on large scales or for industrial applications. These metals are usually rare and expensive, their compounds can be toxic and removing the residues from a process can also be difficult. With increasing economic and environmental awareness, many chemists have kept alive the dream of effecting similar bond-forming reactions but in the absence of transition metals.

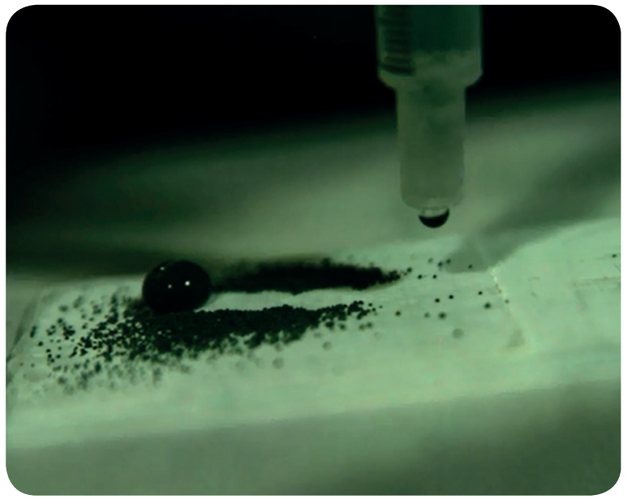
An exciting new project has begun in the lab of Dr Jon Wilden that seeks to investigate the formation of new carbon-carbon and carbon-heteroatom bonds in the absence of transition metal mediators. Recently funded by the EPSRC, the project aims to build on early observations from the Wilden lab that suggest that simple alkoxide bases (some of which have been known for centuries) can promote certain bond-forming reactions previously thought to be the preserve of transition metal catalysis. Preliminary results suggest that under certain circumstances group 1 alkoxide bases (particularly potassium alkoxides) can behave as single electron donors, initiating radical reactions in various organic substrates leading to new bonds being formed. Early results show that for certain substrates, by carefully controlling the conditions, new bonds can be created with efficiencies similar to those observed for their 'classical' organometallic counterparts.

The ultimate goal, to effect carbon-carbon bond formation in an efficient, sustainable and environmentally benign manner is still a long way off, however this research project will seek to realize this ambition by exploring this exciting and fast moving field.

Water behaves like jelly, this is not magic. (Yao Lu)

This is SCIENCE!!!





Dirt is removed by a rolling water droplet on the painted superhydrophobic surface (Yao Lu/UCL)

Many surfaces in nature have super-water-repellent (superhydrophobic) self-cleaning properties, such as the lotus plant and water strider legs. Water forms near spherical shapes that roll on the surface; the rolling motion picks up and removes dirt, viruses, and bacteria. To achieve near spherical water droplets, the surfaces must be highly textured combined with extremely low water affinity. However, artificial superhydrophobic surfaces are mechanically weak and stop functioning when exposed to oil. In this work, we have created an ethanolic suspension of perfluorosilane-coated titanium dioxide nanoparticles that forms a paint that can be applied on both hard and soft substrates to create a self-cleaning surface that functions even upon immersion in oil. Commercial adhesives were used to bond the paint to various substrates and promote robustness. These surfaces maintained their water repellency after finger-wipe, knife-scratch, and even 40 abrasion cycles with sandpaper. The formulations developed can be used on clothes, paper, glass, and steel for a myriad of self-cleaning applications.

For details please refer to **Yao Lu, Sanjayan Sathasivam, Jinlong Song, Colin R. Crick, Claire J. Carmalt, and Ivan P. Parkin, Robust self-cleaning surfaces that function when exposed to either air or oil, *Science* 347, 1132 (2015). DOI: 10.1126/science.aaa0946.**

RESEARCH HIGHLIGHTS

Support morphology affects nanoparticle adsorption

Dr. Alistair Holdsworth and
Prof. Jawwad Darr

Chi-Ming Yim, working as a postdoc in Geoff Thornton's group, has discovered an intriguing phenomenon in adsorption properties of nanoparticles. Low temperature scanning tunnelling microscopy (STM) experiments, carried out in the LCN, have allowed direct imaging of carbon monoxide molecular over layers formed on the palladium nanoparticles themselves supported on a titania substrate. Measurements of molecular orientation on a single nanoparticle using facilities at the Diamond Light Source indicate that the molecules behave in the same way as on a single crystal surface. However, with the higher spatial resolution of STM, Pd nanoparticles can be seen to grow like a carpet over substrate step-edges giving rise to a curved top facet (see Figure). Yim found that on the curved top facet of the nanoparticle, the adsorption behaviour of CO molecules is found to differ from that on single crystal surfaces. Theoretical calculations suggest that this is caused by strain, induced to the particle surface during the carpet growth.

This result has important implications beyond our basic understanding of the chemistry taking place on supported nanoparticles. This support morphology effect will have a decisive impact on the rate of chemical reactions. It also suggests a method of tuning the reactivity of multi-component systems by designing nanoparticle/substrate interfaces.

Geoff Thornton, coordinator of the project said " In this work we have combined world class experimental facilities at Diamond Light Source and the LCN as well as cutting edge calculations to unearth a key role of an oxide support in heterogeneous catalysis. The metal nanoparticles, which form the active ingredient of a catalyst are structurally distorted in a subtle manner to change the way that they interact with reactants and products in the catalyst. With this knowledge we can design the metal support to maximise the efficiency, reducing the amount of the expensive metal needed in, for instance, your automobile catalytic converter."

The work was supported by a European Research Council Advanced Grant entitled "EnergySurf" as well an Engineering & Physical Science Research Council NextGeneration grant.

Chemistry Author(s):

Geoff Thornton

Other contributors:

Chi Ming Yim, Coinneach Dover, Chi Pang, Christopher Muryn (Manchester), Francesco Macherrozzi, Sarnjeet Dhesi (Diamond Light Source), Diego Hermoso, Rubén Pérez (U Autonoma, Madrid)

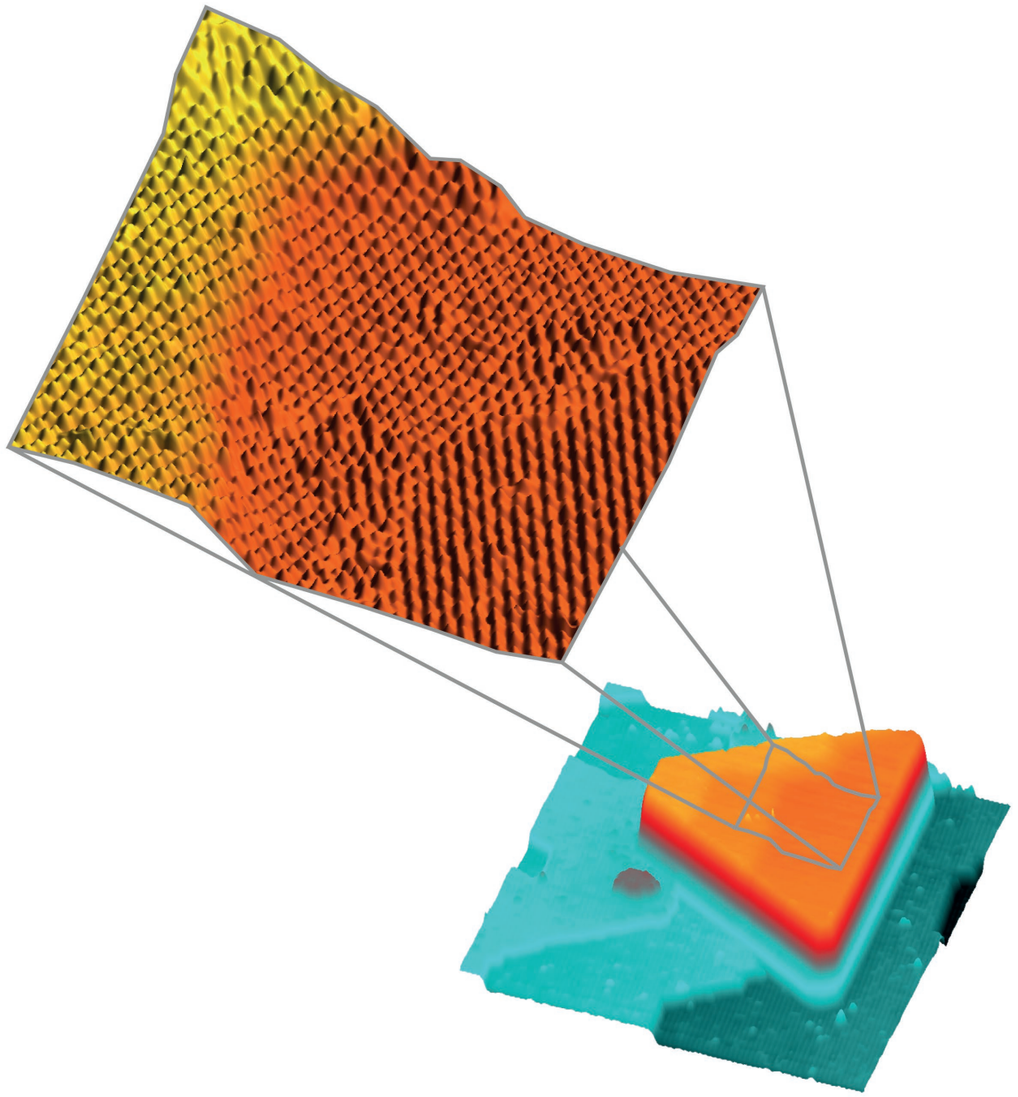


Figure: 3D STM micrograph showing a Pd nanocrystal curving across the step edge of the titania support in a carpet-like manner. On the curved top facet of the nanocrystal, the adsorption behavior of CO molecules (imaged as bright features) differs from that of the single crystal surface

GRANTS AND AWARDS

New Grants and Awards

Super Resolution Imaging for Cell Biology and Neuroscience at UCL
£50,000
MRC
PI: Professor Giuseppe Battaglia
01-Sep-14

First Principles Design of Novel Ammonia Synthesis Catalysts
£322,480
EPSRC
PI: Prof Richard Catlow
01-Sep-14

GRAPHENE : Graphene-based Revolutions in ICT and Beyond
£84,070
EUROPEAN COMMISSION FP7
PI: Prof Paul McMillan
01-Oct-14

MIIA (Materials Innovation Impact Acceleration) Award: Maximising Impact of a new continuous pilot for UK Catalysis
£10,000
ILIKA TECHNOLOGIES LTD
PI : Prof Jawwad Darr
01-Oct-14

SUSTAINABLE OXIDATION CATALYSTS FOR THE PRODUCTION OF SOLAR HYDROGEN AND CHLORINE FROM BRINE
569,522.13
EPSRC
PI : Prof Jawwad Darr
01-Oct-14

Quantum Technologies 2014/2015
£21,723
EPSRC
PI: Prof Peter Coveney
01-Oct-14

ICE Glazing: Intelligent Coatings for Energy-Efficient Glazing
£435,724
EPSRC
PI: Prof Gopinathan Sankar
01-Oct-14

Artist in Residence
£15,000
LEVERHULME TRUST
PI: Prof Julian Evans
01-Oct-14

CSP Modelling of Flexible Molecules: Assessing Crystallizability
£95,016
ELI LILLY AND COMPANY LTD
PI: Prof Sarah (Sally) Price
01-Nov-14

Development of Industry-Ready Technology for the Construction of Next Generation Antibody Therapeutics
£25,000
NATIONAL INSTITUTE FOR HEALTH RESEARCH UNIVERSITY COLLEGE LONDON HOSPITALS BIOMEDICAL RESEARCH CENTRE
PI: Mr. Vijay Chudasama
01-Dec-14

WTISSF 3: Institutional Strategic Support Fund (ISSF)Third Tranche
£25,000
WELLCOME TRUST
PI: Mr. Vijay Chudasama
01-Dec-14

Tailoring the Atomic Structure of Advanced Sol-Gel Materials for Regenerative Medicine through High-Performance Computing
£202,522
EPSRC
PI: Dr Antonio Tilocca
01-Jan-15

ELEVATE : Electrochemical Vehicle Advanced Technology
£200,516
EPSRC
PI : Prof Jawwad Darr
01-Jan-15

SUPERSOLAR : Solar Energy Hub
£121,960
EPSRC
PI: Dr Robert Palgrave
01-Feb-15

EUDAT2020
£129,500
EUROPEAN COMMISSION HORIZON 2020
PI: Prof Peter Coveney
01-Mar-15

Optimisation of a Semi-Synthetic Ligation Strategy for Single Glycoform
£349,134
BBSRC
PI: Dr Derek Macmillan
01-Mar-15

New strategies for the Preparation and Stabilisation of Amorphous Pharmaceuticals
£14,529
ROYAL SOCIETY
PI: Dr Christoph Salzmann
01-Mar-15

Perovskite Structured Thermoelectric Materials
£12,000
ROYAL SOCIETY
PI: Prof Gopinathan Sankar
01-Mar-15

ICES: From Molecular Cloud to Ocean
£105,166
STFC
PI: Prof Stephen Price
01-Apr-15

Advanced Flow Technology for Healthcare Materials Manufacturing
£419,844
EPSRC
PI: Prof Ivan Parkin
01-Apr-15

Predicting Drug-Target Binding Kinetic through Multi-Scale Simulations
£245,251
EPSRC
PI: Prof Francesco Luigi Gervasio
01-Apr-15

Electrodes by Design – Microstructural Engineering of High Performance Electrodes for Solid Oxide Fuel Cells
£133,935
EPSRC
PI : Prof Jawwad Darr
01-May-15

New Frontiers in Transition Metal Free Synthesis
£345,140
EPSRC
PI: Dr Jon Wilden
01-May-15

Personalised Drug Selection for Cancer Treatment in Qatar
£170,319
QATAR NATIONAL RESEARCH FUND
PI: Prof Peter Coveney
01-Jul-15

Opening the Door to Novel Antibody Fragment-based Therapeutics and Diagnostics Via a "Dual Click" Strategy
£421,506
EPSRC
PI: Prof Stephen Caddick
01-Jul-15

Abdollah MR, Kalber T, Tolner B, Southern P, Bear JC, Robson M, Pedley RB, **Parkin IP,** Pankhurst QA, Mulholland P, Chester K, **Prolonging the circulatory retention of SPIONs using dextran sulfate: in vivo tracking achieved by functionalisation with near-infrared dyes.** Faraday discussions, (2014) 175, 41-58.

Abraham MH, Abraham RJ, AcreeWE, **Aliev AE,** Leo AJ, Whaley WL, **An NMR method for the quantitative assessment of intramolecular hydrogen bonding;** application to physicochemical, environmental, and biochemical properties. Journal of Organic Chemistry, (2014) 79, 11075-11083.

Al-Hamdani YS, Alfe D, von Lilienfeld OA, **Michaelides A, Water on BN doped benzene: A hard test for exchange-correlation functionals and the impact of exact exchange on weak binding.** Journal of Chemical Physics, (2014) 141. 18C530

Ali TT, Narasimharao K, **Parkin IP,** Carmalt CJ, Sathasivam S, Basahel SN, Bawaked SM, Al-Thabaiti SA, **Effect of pretreatment temperature on the photocatalytic activity of microwave irradiated porous nanocrystalline ZnO.** New Journal of Chemistry, (2015) **39**, 321-332.

Aliev AE, Arendorf JR, Pavlakos I, Moreno RB, **Porter MJ,** Rzepa HS, **Motherwell WB, Surfing the π-clouds for Non-covalent Interactions: A comparative Study of Arenes versus Alkenes.** Angewandte Chemie International Edition, (2015). **54**(2):551-5

Aliev AE, Pavlakos I, Arif T, **Motherwell WB,** Tizzard GJ, Coles SJ, **Lone Pair (No-π!) Heteroarene Noncovalent Interactions: the Janus faced Hydroxyl Group.** Angewandte Chemie International Edition, (2015). **54**, 8169-8174

Al-Jibori SA, Al-Nassiry RAQ, Al-Jibori GHH, Merzweiler K, Wagner C, Schmidt H, Basak-Modi S, **Hogarth G, Palladium(II) saccharinate complexes trans-[Pd(sac)(2)(LH)(2)] with amino- and acetylamino-pyridine co-ligands: molecular structures of trans-[PdCl2(2-ampyH)(2)].2dmf (2-ampyH=2-amino-3-methylpyridine) and trans-[Pd(kappa(2)-2-acmpy (2)] (2-acmpyH=2-acetylamino-3-methylpyridine)**, Transition Metal Chemistry, (2014) **39**, 735-740.

Allen JP, Galea NM, Watson GW, **Palgrave RG,** Kahk JM, Payne DJ, Robinson MDM, Field G, Regoutz A, Egdell RG, **Valence States in CeVO4 and Ce0.5Bi0.5VO4 Probed by Density Functional Theory Calculations and X-ray Photoemission Spectroscopy,** Journal of Physical Chemistry C, (2014) **118**, 25330-25339.

Anderson JC, Campbell IB, Campos S, Shannon **J, Tocher DA, Stereoselective synthesis of 1,2-diamine containing indolines by a conjugate addition nitro-Mannich reaction.** Organic & Biomolecular Chemistry, (2015) **13,** 170-177.

Anderson JC, Kalogirou AS, Tizzard GJ, **Conjugate addition nitro-Mannich reaction of carbon and heteroatom nucleophiles to nitroalkenes.** Tetrahedron, (2014).**70**, 9337-9351

Anderson JC, Shannon J, Campbell IB, Campos S, **Diastereoselective synthesis of β-aminosulfones from the 1,2-addition to N-(para-methoxyphenyl) imines.** Tetrahedron Letters, (2014) **55**, 7206-7208.

Andreoli D, **Volpe G**, Katz O, Gigan S, Popoff S, Grésillon S, **Deterministic control of broadband light through a multiply scattering medium via the multispectral transmission matrix.** Scientific Reports, (2015) **5**. 10347

Asara GG, **Roldan A**, Ricart JM, Rodriguez JA, Illas F, **de Leeuw NH**, **New Insights into the Structure of the C-Terminated beta-Mo2C (001) Surface from First-Principles Calculations.** Journal of Physical Chemistry C, (2014) **118**, 19224-19231.

Aschauer UJ, **Tilocca A**, Selloni A, **Ab initio simulations of the structure of thin water layers on defective anatase TiO2 (101) surfaces.** International Journal of Quantum Chemistry, (2015) **115**, 1250-1257

Aziz A, **Hailes HC**, Ward JM, **Evans JRG, Long-term stabilization of reflective foams in sea water.** RSC Advances, (2014) **4**, 53028-53036.

Barnes P, Jupe AC, Jacques SDM, O'Connor D, Johnson M, Hooper DP, Colston SL, **Catlow CRA, Sankar G, Bell R, McMillan PF, Energy-dispersive (powder) diffraction.** Journal of Research of National Institute Standards & Technology, (2015).

Bayliss RD, Cabana J, Fearn S, Kilner JA, Skinner SJ, Cook SN, **Scanlon DO**, Greaves C, **Understanding the defect chemistry of alkali metal strontium silicate solid solutions: Insights from experiment and theory.** Journal of Materials Chemistry A,(2014) 2, 17919-17924.

Beale AM, Gao F, Lezcano-Gonzalez I, Peden CH, Szanyi J, **Recent advances in automotive catalysis for NOx emission control by small-pore microporous materials.** Chemical Society Reviews, (2015).

Beale AM, Jacques SDM, Gibson EK, Di Michiel M, **Progress towards five dimensional diffraction imaging of functional materials under process conditions.** Coordination Chemistry Reviews, (2014) **277**, 208-223.

Beale AM, Lezcano-Gonzalez I, Maunula T, **Palgrave RG, Development and characterization of thermally stable supported V–W–TiO 2 catalysts for mobile NH 3 –SCR applications** Catalysis, Structure & Reactivity, (2015) **1**, 25-34.

Bear JC, Dunnill CW, Peveler WJ, **Parkin IP**, McNaughter PD, O'Brien P, **Nanoparticle-sulphur "inverse vulcanisation" polymer composites.** Chemical Communications, (2015) **51**, 10467-10470.

Bear JC, Hollingsworth N, Roffey A, Hogarth G, **Parkin IP**, Mcnaughter PD, Mayes AG, Macdonald TJ, Nann T, Ng WH, Kenyon AJ, **Doping Group IIB Metal Ions into Quantum Dot Shells via the One-Pot Decomposition of Metal-Dithiocarbamates.** Advanced Optical Materials, (2015) **3**, 704-712.

Bear JC, Yu B, Blanco-Andujar C, McNaughter PD, Southern P, Mafina MK, Pankhurst QA, **Parkin IP, A low cost synthesis method for functionalised iron oxide nanoparticles for magnetic hyperthermia from readily available materials.** Faraday Discuss, (2014) **175**, 83-95.

Beatrup D, Wade J, Biniek L, **Bronstein H**, Hurhangee M, Kim JS, McCulloch I, Durrant J, **Polaron stability in semiconducting polymer neat films.** Chemical Communications, (2014) **50**, 14425-14428.

Beech SJ, Noimark S, Page K, Noor N, Allan E, **Parkin IP, Incorporation of crystal violet, methylene blue and safranin O into a copolymer emulsion; the development of a novel antimicrobial paint.** RSC Advances, (2015) **5**, 26364-26375.

Berardo E, Hu H-S, van Dam HJJ, Shevlin SA, **Woodley SM**, Kowalski K, **Zwijnenburg MA, Describing Excited State Relaxation and Localization in TiO2 Nanoparticles Using TD-DFT.** Journal of Chemical Theory And Computation, (2014) **10**, 5538-5548.

Berardo E, **Zwijnenburg MA, Modeling the Water Splitting Activity of a TiO2 Rutile Nanoparticle.** The Journal of Physical Chemistry C, (2015) **119**, 13384-13393.

Bhachu DS, Saban EJ, **Bronstein H, Parkin IP,** Carmalt CJ, Palgrave RG, **Scanlon DO, Scalable route to CH 3 NH 3 PbI 3 perovskite thin films by aerosol assisted chemical vapour deposition.** Journal of Materials Chemistry A, (2015) **3**, 9071-9073.

Bhachu DS, **Sankar G**, Knapp CE, **Carmalt CJ**, **Parkin IP**, **Scanlon DO**, Cibin G, Dent AJ, Veal TD, Egdell RG, **Origin of high mobility in molybdenum-doped indium oxide.** Chemistry of Materials, (2015) **27**, 2788-2796.

Bhachu DS, Sathasivam S, **Carmalt CJ**, **Parkin IP**, **Sankar G**, **Scanlon DO**, Cibin G, Watson GW, Bawaked SM, Obaid AY, Al-Thabaiti S, Basahel SN, **Solution processing route to multifunctional titania thin films: Highly conductive and photcatalytically active Nb:TiO.** Advanced Functional Materials, (2014) **24**, 5075-5085.

Blake MP, **Kaltsoyannis N**, Mountford P, **Synthesis, molecular and electronic structure, and reactions of a Zn-Hg-Zn bonded complex.** Chemical Communications, (2015) **51**, 5743-5746.

Boldrin D, Fak B, Enderle M, Bieri S, Ollivier J, Rols S, Manuel P, **Wills AS**, **Haydeeite: a spin-1/2 kagome ferromagnet.** Physical Review B, (2015) 91.

Boldrin D, **Wills AS**, **SrCu3V2O8(OH)(2) - dynamic Jahn-Teller distortions and orbital frustration in a new S=1/2 kagome antiferromagnet.** Journal of Materials Chemistry C, (2015) **3**, 4308-4315.

PUBLICATIONS

Borgdorff J, Ben Belgacem M, Bona-Casas C, Fazendeiro L, Groen D, Hoenen O, Mizeranschi A, Suter JL, Coster D, **Coveney PV**, Dubitzky W, Hoekstra AG, Strand P, Chopard B, **Performance of distributed multiscale simulations.** Philosophical transactions. Series A, Mathematical, physical, and engineering sciences, (2014) **372**.

Borgdorff J, Hoekstra AG, Mamonski M, Bosak B, Kurowski K, Ben Belgacem M, Chopard B, Groen D, **Coveney PV**, **Distributed multiscale computing with MUSCLE 2, the Multiscale Coupling Library and Environment.** Journal of Computational Science, (2014) **5**, 719-731.

Bovis MJ, Woodhams JH, MacRobert AJ, Noimark S, Peveler WJ, **Parkin IP**, Kay CWM, Weiner J, Correia A, Wilson M, Allan E, **Photosensitisation studies of silicone polymer doped with methylene blue and nanogold for antimicrobial applications.** RSC Advances, (2015) **5**, 54830-54842.

Bromley ST, Goumans TPM, Herbst E, Jones AP, **Slater B**, **Challenges in modelling the reaction chemistry of interstellar dust.** Physical Chemistry Chemical Physics, (2014) **16**, 18623-18643.

Bronstein HA, Andernach RE, Rossbauer S, Ashraf RS, Faber H, Anthopoulos TD, Mcculloch I, Heeney M, **Conjugated polymer-porphyrin complexes for organic electronics.** ChemPhysChem, (2015) **16**, 1223-1230.

Brookes C, Wells PP, Dimitratos N, Jones W, Gibson EK, Morgan DJ, Cibin G, Nicklin C, Mora-Fonz D, **Scanlon DO**, **Catlow CRA**, Bowker M, **The Nature of the Molybdenum Surface in Iron Molybdate. The Active Phase in Selective Methanol Oxidation.** Journal of Physical Chemistry C, (2014) **118**, 26155-26161.

Brown NJ, García-Trenco A, Weiner J, White ER, Allinson M, Chen Y, Shaffer MSP, Williams CK, Wells PP, **Gibson EK**, Hellgardt K, **From organometallic zinc and copper complexes to highly active colloidal catalysts for the conversion of CO2 to methanol.** ACS Catalysis, (2015) **5**, 2895-2902.

Bučar D-K, Cockcroft JK, Elliott JA, Eddleston MD, Jones W, **Sonocrystallization yields monoclinic paracetamol with significantly improved compaction behaviour.** Angewandte Chemie - International Edition. (2015) **54**, 249-253.

Bučar D-K, Lancaster RW, Bernstein J, **Disappearing Polymorphs Revisited.** Angewandte Chemie - International Edition, (2015) **54**, 6972-6993.

Bučar D-K, Macgillivray LR, Henry RF, Zhang GGZ, **Synthon hierarchies in crystal forms composed of theophylline and hydroxybenzoic acids: Cocrystal screening via solution-mediated phase transformation.** Crystal Growth and Design, (2014) **14**, 5318-5328.

Buckeridge J, **Catlow CRA**, Logsdail AJ, **Scanlon DO**, Shevlin SA, **Woodley SM**, Sokol AA, Butler KT, Walsh A, **Polymorph Engineering of TiO2: Demonstrating How Absolute Reference Potentials Are Determined by Local Coordination.** Chemistry of Materials, (2015) **27**, 3844-3851.

Buckeridge J, **Catlow CRA**, **Scanlon DO**, Keal TW, Sherwood P, Miskufova M, Walsh A, **Woodley SM**, Sokol AA, **Determination of the nitrogen vacancy as a shallow compensating center in GaN doped with divalent metals.** Physical Review Letters, (2015) **1**.

Buffet J-C, Wanna N, Arnold TAQ, Gibson EK, Wells PP, Wang Q, Tantirungrotechai J, O'Hare D, **Highly Tunable Catalyst Supports for Single-Site Ethylene Polymerization.** Chemistry of Materials, (2015) **27**, 1495-1501.

Bunney TD, Wan S, Thiyagarajan N, Sutto L, Williams SV, Ashford P, Koss H, Knowles MA, Gervasio FL, **Coveney PV**, Katan M, **The Effect of Mutations on Drug Sensitivity and Kinase Activity of Fibroblast Growth Factor Receptors: A Combined Experimental and Theoretical Study.** EBioMedicine, (2015) **2**,194-204.

Burke DJ, Puletti F, Brown WA, Woods PM, Viti S, **Slater B**, **Glycolaldehyde, methyl formate and acetic acid adsorption and thermal desorption from interstellar ices.** Monthly Notices of The Royal Astronomical Society, (2015) **447**, 1444-1451.

Burns JR, Al-Juffali N, Janes SM, **Howorka S, Membrane-spanning DNA nanopores with cytotoxic effect.** Angewandte Chemie International Edition, (2014) **53**, 12466-12470.

Butchosa C, Guiglion P, **Zwijnenburg MA**, **Carbon Nitride Photocatalysts for Water Splitting: A Computational Perspective.** Journal of Physical Chemistry C, (2014) **118**, 24833-24842.

Byun J, **Patel HA**, Yavuz CT, **Magnetic BaFe12O19 nanofiber filter for effective separation of Fe3O4 nanoparticles and removal of arsenic.** Journal of Nanoparticle Research, (2014) **16**.

Cavalli A, Spitaleri A, Saladino G, **Gervasio FL, Investigating drug-target association and dissociation mechanisms using metadynamics-based algorithms.** Accounts of Chemical Research, (2014) **48**, 277-285.

Chadwick NP, Sathasivam S, Bawaked SM, Mokhtar M, Althabaiti SA, Basahel SN, **Parkin IP, Carmalt CJ**, **The use of time resolved aerosol assisted chemical vapour deposition in mapping metal oxide thin film growth and fine tuning functional properties.** Journal of Materials Chemistry A, (2015) **3**, 4811-4819.

Chatzidaki A, Gill-Thind JK, Millar NS, D'Oyley JM, **Sheppard TD, The influence of allosteric modulators and transmembrane mutations on desensitisation and activation of α7 nicotinic acetylcholine receptors.** Neuropharmacology, (2015) **97**, 75-85.

Chen F, Xu W, Song J, Huang S, Wang L, Liu X, Lu Y, **Parkin IP**, **Hydrophilic patterning of superhydrophobic surfaces by atmospheric-pressure plasma jet.** Micro and Nano Letters, (2015) **10**, 105-108.

Chen S, Noor N, **Parkin IP**, Binions R, **Temperature and thickness-dependent growth behaviour and opto-electronic properties of Ga-doped ZnO films prepared by aerosol-assisted chemical vapour deposition.** Journal of Materials Chemistry A, (2014) **2**, 17174-17182.

Christie JK, Ainsworth RI, **de Leeuw NH**, **Ab initio molecular dynamics simulations of structural changes associated with the incorporation of fluorine in bioactive phosphate glasses.** Biomaterials, (2014) **35**, 6164-6171.

Chudasama V, **Pentafluorophenyl vinyl sulfonate enables efficient, metal-free, radical-based alkene hydroacylation with an aldehyde as a limiting reagent.** RSC Advances, (2015) **5**, 44423-44426.

Coggins AJ, **Tocher DA, Powner MW**, **One-step protecting-group-free synthesis of azepinomycin in water.** Organic and Biomolecular Chemistry, (2015) **13**, 3378-3381.

Cowper B, Shariff L, Chen W, Gibson SM, Di WL, **Macmillan D**. **Expanding the scope of N → S acyl transfer innative peptide sequences.** Organic & biomolecular chemistry, (2015) **13**, 7469-7476.

Cowper B, Sze TM, Premdjee B, White AFB, Hacking A, **Macmillan D, Examination of mercaptobenzyl sulfonates as catalysts for native chemical ligation: application to the assembly of a glycosylated Glucagon-Like Peptide 1 (GLP-1) analogue.** Chemical Communications, (2015) **51**, 3208-3210.

Crick CR, Bhachu DS, **Parkin IP**, **Superhydrophobic silica wool-a facile route to separating oil and hydrophobic solvents from water.** Science And Technology of Advanced Materials, (2014) **15**.

Das NK, Rigby K, **de Leeuw NH**, **The effect of helium nano-bubbles on the structures stability and electronic properties of palladium tritides: a density functional theory study.** Proceedings of The Royal Society A-Mathematical Physical And Engineering Sciences, (2014) **470**, 2171

Davies GB, Krüger T, **Coveney PV**, Harting J, **Detachment energies of spheroidal particles from fluid-fluid interfaces.** J Chem Phys, (2014) **141**, 154902.

Davies GB, Krüger T, **Coveney PV**, Harting J, Bresme F, **Assembling ellipsoidal particles at fluid interfaces using switchable dipolar capillary interactions.** Advanced Materials, (2014) **26**, 6715-6719.

Davies GB, Krüger T, **Coveney PV**, Harting J, Bresme F, **Capillary interactions: assembling ellipsoidal particles at fluid interfaces using switchable dipolar capillary interactions.** Advanced Materials, (2014) **26**.

Deacon-Smith DE, **Scanlon DO**, **Catlow CR**, Sokol AA, **Woodley SM, Interlayer cation exchange stabilizes polar perovskite surfaces.** Advanced Materials, (2014) **26**, 7252-7256.

Deszcz D, Affaticati P, Gegel A, Ward JM, Dalby PA, **Ladkau N**, Hailes HC, **Single active-site mutants are sufficient to enhance serine: Pyruvate α-transaminase activity in an ω-transaminase.** FEBS Journal, (2015).
Deuzing IP, Charpentier C, Wright DW, Matheron S, Paton J, Frentz D, van de Vijver DA, **Coveney PV**, Descamps D, **ANRS CO5 HIV-2 Cohort, Boucher CA, Beerens N, Mutation V111I in HIV-2 reverse transcriptase increases the fitness of the nucleoside analogue-resistant K65R and Q151M viruses.** Journal of Virology, (2015) **89**, 833-843.

Dölker N, Górna MW, Sutto L, Torralba AS, Superti-Furga G, **Gervasio FL**, **The SH2 Domain Regulates c-Abl Kinase Activation by a Cyclin-Like Mechanism and Remodulation of the Hinge Motion** Plos Computational Biology, (2014) **10**, 1003863-1003863.

Doro F, Belvisi L, Civera M, Saladino G, **Gervasio FL**, **New insights into the molecular mechanism of E-cadherin-mediated cell adhesion by free energy calculations.** Journal of Chemical Theory and Computation, (2015) **11**, 1354- 1359.

Du HB, Jia Y, Sun Q, **Guo ZX**, **Single vacancy defects diffusion at theinitial stage of graphene growth: A first-principles study.** Physics Letters, Section A: General, Atomic and Solid State Physics, (2014) **379**, 1270-1273.

Evans GP, Buckley DJ, Skipper NT, **Parkin IP, Single-walled carbon nanotube composite inks for printed gas sensors: Enhanced detection of NO, NH, EtOH and acetone.** RSC Advances, (2014) **4**, 51395-51403.

Evans M, Di Maggio F, **Blackman C**, **Sankar G**, **AACVD synthesis of catalytic gold nanoparticle-modified cerium(IV) oxide thin films.** Physica Status Solidi (C) Current Topics in Solid State Physics, (2015) **12**, 996-1000.

Ficici E, Andricioaei I, **Howorka S**, **Dendrimers in Nanoscale Confinement: The Interplay between Conformational Change and Nanopore Entrance.** Nano letters, (2015) **15**, 4822-4828

Fletcher JD, Parkes MA, **Price SD**, **Bond-forming reactions of N-2(2+) with C2H4, C2H6, C3H4 and C3H6.** International Journal of Mass Spectrometry, (2015) **377**, 101-108.

Forde MM, Armstrong RD, McVicker R, **Dimitratos N**, Jenkins RL, Hammond C, Lopez-Sanchez JA, Hutchings GJ, Wells PP, He Q, Lu L, Kiely CJ, **Light alkane oxidation using catalysts prepared by chemical vapour impregnation: Tuning alcohol selectivity through catalyst pre-treatment.** Chemical Science, (2014) **5**, 3603-3616.

Foster RW, Benhamou L, **Porter MJ**, **Bučar D-K**, **Hailes H**C, **Sheppard TD**, Tame CJ, **Irreversible endo-selective diels-alder reactions of substituted alkoxyfurans: A general synthesis of endocantharimides.** Chemistry - A European Journal, (2015) **21**, 6107-6114

Franco CA, Jones ML, Bernabeu MO, Geudens I, Mathivet T, Rosa A, Lopes FM, Lima AP, Ragab A, Collins RT, Phng L-K, **Coveney PV**, Gerhardt H, **Dynamic Endothelial Cell Rearrangements Drive Developmental Vessel Regression.** Plos Biology, (2015) **13**.

Fullstone G, **Battaglia G**, Wood J, Holcombe M, **Modelling the transport of nanoparticles under blood flow using an agent-based approach.** Scientific Reports, (2015) **5**.

Gadipelli S, **Guo ZX**, **Tuning of ZIF Derived Carbon with High Activity, Nitrogen Functionality, and Yield - A Case for Superior CO2 Capture.** ChemSusChem, (2015) **8**, 2123-2132.

Gadipelli S, Patel HA, **Guo Z**, **An Ultrahigh Pore Volume Drives Up the Amine Stability and Cyclic CO2 Capacity of a Solid-Amine Carbon Sorbent.** Advanced materials, (2015).

Gao M, Wang D, Zhang X, Pan H, Liu Y, Liang C, Shang C, **Guo Z**, **A hybrid Si@ FeSiy/SiOx anode structure for high performance lithium-ion batteries via ammonia-assisted one-pot synthesis.** Journal of Materials Chemistry A, (2015) **3**, 10767-10776.

Ghosh S, **Holt KB**, Kabir SE, Richmond MG, Hogarth G, **Electrocatalytic proton reduction catalysed by the low-valent tetrairon-oxo cluster [Fe-4(CO)(10)(kappa(2)-dppn)(mu(4)-O)](2-) [dppn=1,1'- bis(diphenylphosphino)naphthalene].** Dalton Transactions, (2015) **44**, 5160 5169.

Gianetti TL, Nocton G, Minasian SG, **Kaltsoyannis N**, Kilcoyne ALD, Kozimor SA, Shuh DK, Tyliszczak T, Bergman RG, Arnold J, **Electron localization in a mixed-valence diniobium benzene complex.** Chemical Science, (2015) **6**, 993-1003

Gibson EK, **Beale AM**, **Catlow CRA**, Chutia A, Gianolio D, Gould A, Kroner A, Mohammed KMH, Perdjon M, Rogers SM, Wells PP, **Restructuring of AuPd Nanoparticles Studied by a Combined XAFS/DRIFTS Approach.** Chemistry of Materials, (2015) **27**, 3714-3720

Gill-Thind JK, Millar NS, Dhankher P, D'Oyley JM, **Sheppard TD**, **Structurally similar allosteric modulators of α7 nicotinic acetylcholine receptors exhibit five distinct pharmacological effects.** Journal of Biological Chemistry, (2015) **290**, 3552-3562

Gonzalez-Lopez J, Ruiz-Hernandez SE, Fernandez-Gonzalez A, Jimenez A, **de Leeuw NH**, Grau-Crespo R. **Cobalt incorporation in calcite:Thermochemistry of (Ca, Co)CO3 solid solutions from density functional theory simulations.** Geochimica Et Cosmochimica Acta, (2014) **142**, 205-216.

Goodall JBM, Makwana NM, **Darr JA**, Illsley D, Lines R, **Structure-property-composition relationships in doped zinc oxides: Enhanced photocatalytic activity with rare earth dopants.** ACS Combinatorial Science, (2015) **17**, 100-112.

Goyal P, Krasteva PV, Van Gerven N, Gubellini F, Van den Broeck I, Troupiotis-Tsaïlaki A, Jonckheere W, Péhau-Arnaudet G, Pinkner JS, Chapman MR, Hultgren SJ, **Howorka S**, Fronzes R, Remaut H, **Structural and mechanistic insights into the bacterial amyloid secretion channel CsgG.** Nature, (2014) **516**, 250-253.

Greenwood JB, Miles J, Camillis SD, Mulholland P, Zhang L, Parkes MA, **Hailes HC**, **Fielding HH**, **Resonantly enhanced multiphoton ionization spectrum of the neutral green fluorescent protein chromophore.** Journal of Physical Chemistry Letters, (2014) **5**, 3588-3592.

Grenet L, Grondin P, Coumert K, Karst N, Emieux F, Roux F, Fillon R, Altamura G, Fournier H, Faucherand P, Perraud S, **Experimental evidence of light soaking effect in Cd-free Cu2ZnSn(S,Se)4-based solar cells.** Thin Solid Films, (2014) **564**, 375-378.

Grinter DC, Muryn C, Santos B, Shaw B-J, Mentes TO, Locatelli A, **Thornton G**, **Spectromicroscopy of a Model Water-Gas Shift Catalyst: Gold Nanoparticles Supported on Ceria.** Journal of Physical Chemistry C, (2014) **118**, 19194-19204.

Grinter DC, Pang CL, Muryn CA, Maccherozzi F, Dhesi SS, **Thornton G**, **Characterising ultrathin ceria films at the nanoscale: Combining spectroscopy and microscopy.** Journal of Electron Spectroscopy and Related Phenomena, (2014) **195**, 13-17.

Grinter DC, Woolcot T, Pang C-L, **Thornton G**, **Ordered Carboxylates on TiO 2 (110) Formed at Aqueous Interfaces.** The Journal of Physical Chemistry Letters, (2014) **5**, 4265-4269.

Groen D, Chacra DA, Nash RW, Bernabeu MO, **Coveney PV**, Jaros J, **Weighted decomposition in high-performance Lattice-Boltzmann simulations: Are some lattice sites more equal than others?** Lecture Notes in Computer Science (including subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics), (2014) **8759**, 28-38.

Groen D, Guo X, Grogan JA, **Schiller UD**, Osborne JM, **Software development practices in academia: a case study comparison.** arXiv, (2015). arXiv:1506.05272

Groen D, Zwart SP, **From Thread to Transcontinental Computer:Disturbing Lessons in Distributed Supercomputing.** arXiv, (2015). arXiv:1507.01138

Guerreiro A, **Poma A,** Karim K, Moczko E, Takarada J, de Vargas-Sansalvador IP, Turner N, Piletska E, de Magalhães CS, Glazova N, Serkova A, Omelianova A, Piletsky S, **Influence of surface imprinted nanoparticles on trypsin activity** Advanced Healthcare Materials, (2014) **3**, 1426-1429.

Guiglion P, Butchosa C, **Zwijnenburg MA, Polymeric watersplitting photocatalysts; a computational perspective on the water oxidation conundrum.** Journal of Materials Chemistry A, (2014) **2**, 11996-12004.

Guiglion P, **Zwijnenburg MA**, **Contrasting the optical properties of the different isomers of oligophenylene.** Physical Chemistry Chemical Physics, (2015) **17**, 17854-17863.

Guzman JD, Davies HM, McMahon E, Evangelopoulos D, Mortazavi PN, Munshi T, Maitra A, Bhakta S, Pesnot T, Lamming ED, **Hailes HC**, Barrera DA, Cuca LE, Angell R, Ward JM, Gershater MC, Redmond JM, Needham D, **Tetrahydroisoquinolines affect the whole-cell phenotype of Mycobacterium tuberculosis by inhibiting the ATP-dependent MurE ligase.** Journal of Antimicrobial Chemotherapy, (2015) **70**, 1691-1703.

Hammond C, **Dimitratos N**, Hermans I, **Biomimetic Oxidation with Fe-ZSM-5 and HO? Identification of an Active, Extra-Framework Binuclear Core and an Fe-OOH Intermediate with Resonance-Enhanced Raman Spectroscopy.** ChemCatChem, (2015) **7**, 434-440.

Han X, Morgan Stewart H, Shevlin SA, **Catlow CRA**, **Guo ZX**, **Strain and orientation modulated bandgaps and effective masses of phosphorene nanoribbons.** Nano Letters, (2014) **14**, 4607-4614.

Harrison GT, Spadaro MC, Pang CL, Grinter DC, Yim CM, Luches P, **Thornton G**, **Lepidocrocite-like TiO 2 and TiO 2 (110)–(1 × 2) supported on W(100).** Materials Science and Technology, (2015).

Hazael R, Foglia F, Kardzhaliyska L, Daniel I, Meersman F, **McMillan P**, **Laboratory investigation of high pressure survival in Shewanella oneidensis MR-1 into the gigapascal pressure range.** Frontiers in Microbiology, (2014) **5**.Article 612

Herschy B, Whicher A, Camprubi E, Watson C, Dartnell L, Ward J, **Evans JR**, Lane N, **An origin-of-life reactor to simulate alkaline hydrothermal vents.** Journal of Molecular Evolution, (2014) **79**, 213-227.

Hoekstra J, **Beale AM**, Soulimani F, Versluijs-Helder M, Geus JW, Jenneskens LW, **Base Metal Catalyzed Graphitization of Cellulose: A Combined Raman Spectroscopy, Temperature-Dependent X-ray Diffraction and High-Resolution Transmission Electron Microscopy Study.** The Journal of Physical Chemistry C, (2015) **119**, 10653-10661.

Ho-Kimura S, Moniz SJA, Tang J, **Parkin IP, A Method for Synthesis of Renewable Cu2O Junction Composite Electrodes and Their Photoelectrochemical Properties.** ACS Sustainable Chemistry & Engineering, (2015) **3**, 710-717.

Hollingsworth N, Roffey A, Islam H-U, Mercy M, **Roldan A**, Bras W, **Wolthers M**, **Catlow CRA**, **Sankar G**, Hogarth G, **de Leeuw NH**, **Active Nature of Primary Amines during Thermal Decomposition of Nickel Dithiocarbamates to Nickel Sulfide Nanoparticles.** Chemistry of Materials, (2014) **26**, 6281-6292.

Hossain MA, Tianliang Z, Keat LK, Xianglin L, Prabhakar RR, Batabyal SK, Mhaisalkar SG, Wong LH, **Synthesis of Cu(In,Ga)(S,Se) 2 thin films using an aqueous spray-pyrolysis approach, and their solar cell efficiency of 10.5%.** Journal of Materials Chemistry A, (2015) **3**, 4147-4154.

Hu Y-B, **Wolthers M**, Wolf-Gladrow DA, Nehrke G, **Effect of pH and Phosphate on Calcium Carbonate Polymorphs Precipitated at near-Freezing Temperature.** Crystal Growth & Design, (2015) **15**, 1596-1601.

Huang Q-R, **Kingham JR**, Kaltsoyannis N, **The strength of actinide-element bonds from the quantum theory of atoms-in-molecules.** Dalton Transactions, (2015) **44**, 2554-2566.

Huang Y, Fang J, Omenya F, Chernova NA, Zhang R, Wang Q, Whittingham MS, O'Shea M, Quackenbush NF, Piper LFJ, **Scanlon DO**, **Understanding the stability of MnPO.** Journal of Materials Chemistry A, (2014) **2**, 12827-12834.

Huang Z, Fregoso EC, Dimitrov S, Tuladhar PS, Soon YW, **Bronstein H**, Meager I, Zhang W, McCulloch I, Durrant JR, **Optimisation of diketopyrrolopyrrole:fullerene solar cell performance through control of polymer molecular weight and thermal annealing.** Journal of Materials Chemistry A, (2014) **2**, 19282-19289.

Hull EA, Livanos M, Miranda E, Smith ME, Chester KA, **Baker JR**, **Homogeneous bispecifics by disulfide bridging.** Bioconjugate Chemistry, (2014) **25**, 1395-1401.

Humeres E, de Souza EP, Debacher NA, Moreira RDEF, Lopes CN, Fernández MI, Santaballa JA, Canle ML, Schreiner WH, **Aliev AE**, **Photolysis of phenylalanine in the presence of oxidized carbon nanotubes.** Langmuir, (2015) **31**, 164-170

Itani MA, **Schiller UD**, Schmieschek S, Hetherington J, Bernabeu MO, Coveney PV, **Groen D**, Chandrashekar H, Robertson F, **An automated multiscale ensemble simulation approach for vascular blood flow.** Journal of Computational Science, (2015) **9**, 150-155.

Jiang N, **Woodley SM**, **Catlow CRA**, Zhang X, **Applying a new interatomic potential for the modelling of hexagonal and orthorhombic YMnO3.** Journal of Materials Chemistry C, (2015) **3**, 4787-4793.

Jones W, Su R, **Wells PP**, Shen Y, **Dimitratos N**, Bowker M, Morgan D, Iversen BB, Chutia A, Besenbacher F, Hutchings G, **Optimised photocatalytic hydrogen production using core-shell AuPd promoters with controlled shell thickness.** Physical Chemistry Chemical Physics, (2014) **16**, 26638-26644.

Mansor N, Jorge Sobrido AB, **Cora F**, Gibbs C, Jervis R, **McMillan P**, Wang C, Brett DJ, **Graphitic Carbon Nitride Supported Catalysts for Polymer Electrolyte Fuel Cells.** Journal of Physical Chemistry C, (2014) **118**, 6831-6838.

Tobaldi DM, Pullar RC, Binions R, Jorge Sobrido AB, **McMillan PF**, Saeli M, Seabra MP, Labrincha JA, **Influence of sol counter-ions on the visible light induced photocatalytic behaviour of TiO2 nanoparticles.** Catalysis Science & Technology, (2014) **4**, 2134-2146.

Jungmichel S, Clapperton JA, Lloyd J, Spycher C, Pavic L, Li J, Haire LF, Bonalli M, Lukas C, Lukas J, **MacMillan D**, Stucki M, Smerdon SJ, **Molecular basis of ATM and FHA-dependent Mdc1 dimerisation in response to DNA-damage.** Molecular Cell.

Jurcic M, Peveler WJ, **Parkin IP**, Savory CN, **Scanlon DO**, Kenyon AJ, **The vapour phase detection of explosive markers and derivatives using two fluorescent metal-organic frameworks.** Journal of Materials Chemistry A, (2015) **3**, 6351-6359.

Kalidindi SB, Nayak S, Briggs ME, Jansat S, Katsoulidis AP, Miller GJ, Warren JE, Antypov D, Prestly MR, Mart-Gastaldo C, Rosseinsky MJ, **Corà F**, **Slater B**, **Chemical and structural stability of zirconium-based metal-organic frameworks with large three-dimensional pores by linker engineering.** Angewandte Chemie - International Edition, (2015) **54**, 221-226

Karabasov S, Nerukh D, Hoekstra A, Chopard B, **Coveney PV, Multiscale modelling: approaches and challenges.** Philosophical transactions. Series A, Mathematical, physical, and engineering sciences, (2014) **372**.

Kennedy J, Morgan DJ, Bowker M, **Dimitratos N**, Jones W, **Wells PP**, Lu L, Kiely CJ, **Photocatalytic hydrogen production by reforming of methanol using Au/TiO2, Ag/TiO2 and Au-Ag/TiO2 catalysts.** Energy Materials: Materials Science and Engineering for Energy Systems, (2015) **10,** 35-43.

Kermarrec E, Zorko A, Bert F, Colman RH, Koteswararao B, Bouquet F, Bonville P, Hillier A, Amato A, Tol JV, Ozarowski A, **Wills AS,** Mendels P, **Spin dynamics and disorder effects in the S=1/2 kagome Heisenberg spin-liquid phase of kapellasite.** Physical Review B, (2014) 90, 205103.

Kiely CJ, He Q, Tiruvalam R, **Dimitratos N,** Forde MM, Sankar M, Hutchings GJ, **Assessing and controlling the size, morphology and composition of supported bimetallic catalyst nanoparticles.** Microscopy and Microanalysis, (2014) **20**, 74-75.

Kimber HJ, Ennis CP, **Price SD**, **Single and double addition of oxygen atoms to propyne on surfaces at low temperatures.** Faraday Discussions,(2014) **168**, 167-184.

King FD, Aliev A, Caddick S, Tocher D, The triflic acid mediated reactions of benzo-fused cyclic amides. Tetrahedron, (2014).

King SG, **McCafferty L**, Stolojan V, Silva SRP, **Highly aligned arrays of super resilient carbon nanotubes by steam purification.** Carbon, (2015) **84**, 130-137.

Kirkby OM, Sala M, Balerdi G, de Nalda R, Bañares L, Guérin S, **Fielding HH**, **Comparing the electronic relaxation dynamics of aniline and d 7 -aniline following excitation at 272–238 nm.** Physical Chemistry Chemical Physics, (2015) **17**, 16270-16276.

Knapp B, Bardenet R, Deane CM, Bernabeu MO, **Groen D**, Kuijper B, Lewis J, Bordas R, Bruna M, Cooper J, McInerny G, Osborne J, Pitt-Francis J, Gavaghan D, Fletcher AG, Calderhead B, Minssen T, Paulitschke V, Todoric J, Yates CA, **Ten simple rules for a successful cross-disciplinary collaboration.** PLoS Computational Biology, (2015) **11**.

Ko D, **Patel HA**, Yavuz CT, **Synthesis of nanoporous 1,2,4-oxadiazole networks with high CO 2 capture capacity.** Chemical Communications, (2015) **51**, 2915-2917.

Krueger T, Holmes D, **Coveney PV, Deformability-based red blood cell separation in deterministic lateral displacement devices-A simulation study.** Biomicrofluidics, (2014) **8**. 054114

Ladkau N, Schmid A, Bühler B, **The microbial cell—functional unit for energy dependent multistep biocatalysis.** Current Opinion in Biotechnology, (2014) 30, 178-189.

Lichman BR, Gershater MC, Lamming ED, Pesnot T, Sula A, Keep NH, **Hailes HC**, Ward JM, **Dopamine-first' mechanism enables the rational engineering of the norcoclaurine synthase aldehyde activity profile.** FEBS Journal, (2015) **282,** 1137-1151.

Lichman BR, Lamming ED, Pesnot T, Smith JM, **Hailes HC,** Ward JM, **One-pot triangular chemoenzymatic cascades for the syntheses of chiral alkaloids from dopamine.** Green Chemistry, (2015) **17**, 852-855.

Ling M, **Blackman C**, **Growth mechanism of planar or nanorod structured tungsten oxide thin films deposited via aerosol assisted chemical vapour deposition (AACVD).** Physica Status Solidi (C) Current Topics in Solid State Physics, (2015) **12**, 869-877.

Logan N, Cross AJ, Traynor A, Bozec L, **Parkin IP**, Brett P, **Mesenchymal stem cell response to UV-photofunctionalized TiO 2 coated CoCrMo.** RSC Advances, (2014) **4**, 59847-59857.

Logsdail AJ, Scanlon DO, Catlow CRA, Sokol AA, **Bulk ionization potentials and band alignments from three-dimensional periodic calculations as demonstrated on rocksalt oxides.** Physical Review B, (2014) **90**. 155106

Lu Y, Sathasivam S, Song J, Chen F, Xu W, **Carmalt CJ, Parkin IP, Creating superhydrophobic mild steel surfaces for water proofing and oil-water separation.** Journal of Materials Chemistry A, (2014) **2**, 11628-11634.

Lu Y, Sathasivam S, Song J, Crick CR, **Carmalt CJ, Parkin IP**, **Robust self-cleaning surfaces that function when exposed to either air or oil.** Science, (2015) **347**, 1132-1135

Lübke M, Johnson I, Makwana NM, **Darr JA**, Brett D, Shearing P, Liu Z, **High power TiO2 and high capacity Sn-doped TiO2 nanomaterial anodes for lithium-ion batteries. J**ournal of Power Sources, (2015) **294**, 94-102

Luo W, Sankar M, **Beale AM**, He Q, Kiely CJ, Bruijnincx PCA, Weckhuysen BM, **High performing and stable supported nano-alloys for the catalytic hydrogenation of levulinic acid to gamma-valerolactone.** Nature Communications, (2015) **6.** Article 6540

Macdonald TJ, Mange YJ, Dewi MR, Islam HU, **Parkin IP**, Skinner WM, Nann T, **CuInS2/ZnS nanocrystals as sensitisers for NiO photocathodes.** Journal of Materials Chemistry A, (2015) **3**, 13324-13331.

Makkos E, Kerridge A, **Kaltsoyannis N**, **The importance of second shell effects in the simulation of hydrated Sr 2+ hydroxide complexes.** Dalton Transactions, (2015) 44, 11572-11581.

Makwana NM, Hazael R, **McMillan PF**, **Darr JA, Photocatalytic water disinfection by simple and low-cost monolithic and heterojunction ceramic wafers.** Photochemical and Photobiological Sciences, (2015) **14**, 1190-1196.

Makwana NM, **Quesada-Cabrera R, Parkin IP, McMillan PF, Darr JA,** Mills A, A **simple and low-cost method for the preparation of self-supported TiO-WO ceramic heterojunction wafers.** Journal of Materials Chemistry A, (2014) **2**, 17602-17608.

Malkin TL, Murray BJ, **Salzmann CG**, Molinero V, Pickering SJ, Whale TF, **Stacking disorder in ice I.** Physical Chemistry Chemical Physics, (2015) **17**, 60-76.

Marchand P, Pugh D, **Parkin IP, Carmalt CJ, Synthesis and Structural Characterization of beta-Ketoiminate-Stabilized Gallium Hydrides for Chemical Vapor Deposition Applications.** Chemistry-A European Journal, (2014) **20**, 10503-10513.

Marino KA, Sutto L, **Gervasio FL**, **The Effect of a Widespread Cancer-Causing Mutation on the Inactive to Active Dynamics of the B-Raf Kinase.** Journal of the American Chemical Society, (2015) **137**, 5280-5283.

Marson CM, Histone Deacetylase Inhibitors: Their Structure, Function and Potential to Treat Cancer. Advances in Anti-Cancer Agents in Medicinal Chemistry, 1.72 354-425

Marson CM, Regioselective synthesis of substituted piperidine-2,4-diones and their derivatives via Dieckmann cyclisations. Tetrahedron. **71** 7459-7469

Marson CM, Pteridine-2,4-diamine Derivatives as Radical Scavengers and Inhibitors of Lipoxygenase that can possess Anti-Inflammatory Properties. Future Medicinal Chemistry.

Marson CM, Ferretti P, Prasongchean W, **Discovery of a synthetic inhibitor of peptidylarginine deiminase that inhibits apoptosis of neuronal cells.** European Journal of Neuroscience.

Maruani A, Alom S, Canavelli P, Lee MT, Morgan RE, **Chudasama V**, **Caddick S**, **A mild TCEP-based para-azidobenzyl cleavage strategy to transform reversible cysteine thiol labelling reagents into irreversible conjugates.** Chemical Communicatons, (2015) **51**, 5279-5282.

Maruani A, Smith MEB, **Chudasama V**, **Caddick S**, Miranda E, Chester KA, **A plug-and-play approach to antibody-based therapeutics via a chemoselective dual click strategy.** Nature Communications, (2015) **6**.Article 6645

Maurelli S, Berlier G, Chiesa M, Musso F, **Corà F**, **Structure of the catalytic active sites in vanadium-doped aluminophosphate microporous materials. New evidence from spin density studies.** Journal of Physical Chemistry C, (2014) **118**, 19879-19888.

McCabe EE, **Wills AS**, Chapon L, Manuel P, Evans JSO, **Structural and magnetic characterisation of iron oxyselenides Ce2O2Fe2OSe2 and Nd2O2Fe2OSe2.** Physical Review B, (2014) **90**, 165111.

McCafferty L, Stolojan V, King SG, Zhang W, Haq S, Silva SRP. **Decoration of multiwalled carbon nanotubes with protected iron nanoparticles.** Carbon, (2015) **84**, 47-5.5

Meager I, Ashraf RS, Nielsen CB, Donaghey JE, Huang Z, Durrant JR, McCulloch I, **Bronstein H**, **Power conversion efficiency enhancement in diketopyrrolopyrrole based solar cells through polymer fractionation.** Journal of Materials Chemistry C, (2014) **2**, 8593-8598.

Meager I, Schroeder BC, Nielsen CB, Planells M, **Bronstein H**, Rumer JW, James DI, Ashraf RS, McCulloch I, Nikolka M, Sadhanala A, Sirringhaus H, Hayoz P, Flores J-C, **Thieno[3,2-b]thiophene flanked isoindigo polymers for high performance ambipolar OFET applications.** Advanced Functional Materials, (2014) **24,** 7109-7115.

Messager L, Gaitzsch J, Chierico L, **Battaglia G**, **Novel aspects of encapsulation and delivery using polymersomes.** Current Opionion in Phramacology, (2014) **18**, 104-111.

PUBLICATIONS

Miller TS, Belen Jorge A, **Sella A**, **Cora F,** Shearing PR, Brett DJL, **McMillan PF**, **The use of graphitic carbon nitride based composite anodes for lithium-ion battery applications.** Electroanalysis, (2015). DOI: 10.1002/elan.201500205

Minato T, Kajita S, **Pang CL**, Asao N, Yamamoto Y, Nakayama T, Kawai M, Kim Y, **Tunneling Desorption of Single Hydrogen on the Surface of Titanium Dioxide.** ACS Nano, (2015). 9 (7), 6837–6842

Mireku EA, Mensah AY, Mensah MLK, **Tocher DA**, Habtemariam S, **Antiinflammatory Properties of the Stem-bark of Anopyxis klaineana and its Major Constituent, Methyl Angolensate.** Phytotherapy Research, (2014) **28**, 1855-1860.

Momin A, Carter L, Yang Y, McDonald R, Essafi Labouille S, Nief F, Del Rosal I, **Sella A**, Maron L, Takats J, T**o bend or not to bend: experimental and computational studies of structural preference in Ln(Tp(iPr)2)2 (Ln = Sm, Tm).** Inorganic Chemistry, (2014) **53**, 12066-12075.

Moniz SJ, Shevlin SA, An X, **Guo ZX**, Tang J, **Fe2 O3 -TiO2 nanocomposites for enhanced charge separation and photocatalytic activity.** Chemistry, (2014) **20**, 15571-15579.

Moniz SJA, Martin DJ, Tang J, Shevlin SA, **Guo Z-X**, **Visible-light driven heterojunction photocatalysts for water splitting-a critical review.** Energy and Environmental Science, (2015) **8**, 731-759.

Mooney CRS, Parkes MA, Iskra A, **Fielding HH**, **Controlling Radical Formation in the Photoactive Yellow Protein Chromophore.** Angewandte Chemie-International Edition, (2015) **54**, 5646-5649.

Mora-Fonz D, Buckeridge J, Logsdail AJ, **Scanlon DO**, Sokol AA, **Woodley S**, **Catlow CRA**, **Morphological features and band bending at nonpolar surfaces of ZnO.** Journal of Physical Chemistry C, (2015) **119,** 11598-11611

Morgan RE, **Chudasama V**, Moody P, Smith MEB, **Caddick S**, **A novel synthetic chemistry approach to linkage-specific ubiquitin conjugation.** Organic and Biomolecular Chemistry, (2015) **13**, 4165-4168

Murray BJ, Malkin TL, **Salzmann CG**, **The crystal structure of ice under mesospheric conditions.** Journal of Atmospheric And Solar-Terrestrial Physics, (2015) **127**, 78-82.

Naik AJT, **Parkin IP**, Binions R, **Gas Sensing Studies of a n-n Hetero-Junction Array Based on WO3 and ZnO Composites.** IEEE Sensors Journal, (2014) **14**, 3137-3147.

Nanthamathee C, Ling S, **Slater B**, Attfield MP, **Contradistinct Thermoresponsive Behavior of Isostructural MIL-53 Type Metal-Organic Frameworks by Modifying the Framework Inorganic Anion,** Chemistry of Materials, (2014) **27**, 85-95.

Newton MA, Di Michiel M, Ferri D, Fernàndez-Garcia M, **Beale AM**, Jacques SDM, Chupas PJ, Chapman KW, **Catalytic Adventures in Space and Time Using High Energy X-rays,** Catalysis Surveys from Asia, (2014) **18**, 134-148.

Noimark S, Noor N, **Parkin IP**, Weiner J, Williams CK, Shaffer MSP, Allan E, **Dual-mechanism antimicrobial polymer-ZnO nanoparticle and crystal violet-encapsulated silicone.** Advanced Functional Materials, (2015) **25**, 1367-1373.

Nunes JPM, Morais M, Robinson E, Smith MEB, **Caddick S, Baker JR**, **Chudasama V**, Vassileva V, Rajkumar VS, Pedley RB, **Functional native disulfide bridging enables delivery of a potent, stable and targeted antibody-drug conjugate (ADC),** Chemical Communications, (2015) 51, 10624-10627.

Ozkan E, Allan E, **Parkin IP**, **The antibacterial properties of light-activated polydimethylsiloxane containing crystal violet.** RSC Advances, (2014) **4**, 51711-51715.

Ozkan E, Ozkan FT, **Parkin IP**, Allan E, **The use of zinc oxide nanoparticles to enhance the antibacterial properties of light-activated polydimethylsiloxane containing crystal violet.** RSC Advances, (2015) **5**, 8806-8813.

Ozkan FT, Quesada-Cabrera R, **Parkin IP, Silicalite-1/glass fibre substrates for enhancing the photocatalytic activity of TiO.** RSC Advances, (2015) **5**, 6970-6975.

Page K, Correia A, **Parkin IP**, Wilson M, Allan E, **Light-activated antibacterial screen protectors for mobile telephones and tablet computers.** Journal of Photochemistry and Photobiology A: Chemistry, (2015) **296**, 19-24.

Pang CL, Yurtsever A, Onoda J, Sugimoto Y, **Thornton G**, **(2n×1) Reconstructions of TiO2(011) Revealed by Noncontact Atomic Force Microscopy and Scanning Tunneling Microscopy.** The Journal of Physical Chemistry Part C: Nanomaterials and Interfaces,(2014).

Parmentier A, Shephard JJ, Romanelli G, Senesi R, **Salzmann CG**, Andreani C, **Evolution of Hydrogen Dynamics in Amorphous Ice with Density.** Journal of Physical Chemistry Letters, (2015) **6**, 2038-2042.

Patel HA, Ko D, Yavuz CT, **Nanoporous Benzoxazole Networks by Silylated Monomers, Their Exceptional Thermal Stability, and Carbon Dioxide Capture Capacity.** Chemistry of Materials, (2014) **26**, 6729-6733.

Pavlakos I, Arif T, **Aliev AE**, **Motherwell WB,** Tizzard GJ, Coles SJ, **Noncovalent Lone Pair...(No-π!)-Heteroarene Interactions: The Janus-Faced Hydroxy Group.** Angewandte Chemie, (2015) **54**, 8169-8174.

Payongsri P, Dalby PA, Steadman D, **Hailes HC**, **Second generation engineering of transketolase for polar aromatic aldehyde substrates.** Enzyme and Microbial Technology, (2015) **71**, 45-52.

Pesce G, **Volpe G**, Marago OM, Jones PH, Gigan S, Sasso A, Volpe G, **Step-by-step guide to the realization of advanced optical tweezers.** Journal of The Optical Society of America B-Optical Physics, (2015) **32**, 84-98.

Pesce G, Volpe G, Volpe G, Sasso A, **Long-term influence of fluid inertia on the diffusion of a Brownian particle.** Physical Review E, (2014) **90**. 042309

Peveler WJ, **Bear JC,** Southern P, **Parkin IP**, **Organic–inorganic hybrid materials: nanoparticle containing organogels with myriad applications.** Chemical Communications, (2014) **50**, 14418-14420.

Picard A, Testemale D, Wagenknecht L, **Hazael R,** Daniel I, **Iron reduction by the deep-sea bacterium Shewanella profunda LT13a under subsurface pressure and temperature conditions.** Frontiers in Microbiology, (2015) **5**. 796

Ponja SD, **Parkin IP**, **Carmalt CJ**, **Magnesium Oxide Thin Films with Tunable Crystallographic Preferred Orientation via Aerosol-Assisted CVD.** Chemical Vapor Deposition, (2015) **21**, 145-149.

Potter ME, Paterson AJ, Raja R, Mishra B, Kelly SD, Bare SR, **Corà F**, Levy AB, **Spectroscopic and Computational Insights on Catalytic Synergy in Bimetallic Aluminophosphate Catalysts.** Journal of the American Chemical Society, (2015) **137**, 8534-8540.

Price LS, McMahon JA, Lingireddy SR, Lau S-F, Diseroad BA, **Price SL**, Reutzel-Edens SM, **A molecular picture of the problems in ensuring structural purity of tazofelone.** Journal of Molecular Structure, (2014) **1078**, 26-42.

Price SD, Fletcher JD, **Parkes MA**, **Electron transfer and bond-forming reactions following collisions of I2+ with CO and CS2.** Molecular Physics: an international journal in the field of chemical physics. (2015) DOI: 10.1080/00268976.2015.1007105

Price SL, CHEMISTRY Lattice energy, nailed? SCIENCE, (2014) **345**, 619-620.

Price SWT, Ignatyev K, Geraki K, Basham M, Filik J, Vo NT, Witte PT, **Beale AM**, Mosselmans JFW, **Chemical imaging of single catalyst particles with scanning mu-XANES-CT and mu-XRF-CT.** Physical Chemistry Chemical Physics, (2015) 17, 521-529.

Qin HJ, Zakeri K, Ernst A, Sandratskii LM, Buczek P, Marmodoro A, Chuang T-H, **Zhang Y,** Kirschner J, **Long-living terahertz magnons in ultrathin metallic ferromagnets.** Nature Communications, (2015) **6**. 6126

Quesada-Cabrera R, **McMillan PF**, Meersman F, Filinchuk Y, Nies E, Dmitriev V, **Exploring the pressure-temperature behaviour of crystalline and plastic crystalline phases of N-isopropylpropionamide.** CrystEngComm, (2015) **17**, 2562-2568.

Quesada-Cabrera R, Sotelo-Vazquez C, **Darr JA**, **Parkin IP**, **Critical influence of surface nitrogen species on the activity of N-doped TiO thin-films during photodegradation of stearic acid under UV light irradiation.** Applied Catalysis B: Environmental, (2014) **160**, 582-588.

Quirk JB, Rasander M, McGilvery CM, **Palgrave R**, Moram MA, **Band gap and electronic structure of MgSiN2.** Applied Physics Letters, (2014) **105**.112108

Rahaman A, Alam FR, Hossain MK, Abdel-Magied AF, Ghosh S, **Tocher DA**, Haukka M, Kabir SE, Nordlander E, Hogarth G, **Phosphine addition to the sigma,pi-thienyl complex [Fe-2(CO)(6)(mu-Th)(mu-PTh2)] (Th = C4H3S): Carbonyl substitution and migratory carbonyl insertion to give the thienyl-acyl complexes [Fe-2(CO)(4)(diphosphine)(mu-O=C-Th)(mu-PTh2)].** Inorganica Chimica Acta, (2015) **430**, 208-215.

Richter N, Simon RC, Lechner H, Kroutil W, Ward JM, **Hailes HC**, **ω-Transaminases for the amination of functionalised cyclic ketones.** Organic & biomolecular chemistry, (2015).13, 8843-8851

Rios-Solis L, Morris P, Grant C, Odeleye AOO, Ward JM, Dalby PA, Baganz F, Lye GJ, **Hailes HC**, **Modelling and optimisation of the one-pot, multi-enzymatic synthesis of chiral amino-alcohols based on microscale kinetic parameter determination.** Chemical Engineering Science, (2015) **122**, 360-372.

Robinson BW, Tighe CJ, Gruar RI, Mills A, **Parkin IP**, Tabecki AK, Lovelock HLDV, **Darr JA, Suspension plasma sprayed coatings using dilute hydrothermally produced titania feedstocks for photocatalytic applications.** Journal of Materials Chemistry A, (2015) **3**, 12680-12689.

Rogers SM, **Catlow CRA**, Chan-Thaw CE, Gianolio D, Gibson EK, Gould AL, Jian N, Logsdail AJ, Palmer RE, Prati L, Dimitratos N, Villa A, Wells PP, **Tailoring Gold Nanoparticle Characteristics and the Impact on Aqueous-Phase Oxidation of Glycerol. ACS Catalysis,** (2015) **5**, 4377-4384.

Roldan A, Hollingsworth N, Roffey A, Islam H-U, Goodall JBM, **Catlow CRA**, **Darr JA**, **Sankar G**, **Holt KB**, Hogarth G, **De Leeuw NH**, Bras W, **Bio-inspired CO2 conversion by iron sulfide catalysts under sustainable conditions.** Chemical Communications, (2015) **51,** 7501- 7504.

Romero L, Jorge-Sobrido A-B, **McMillian PF**, Binions R, **On titanium dioxide thin films growth from the direct current electric field assisted chemical vapour deposition of titanium (IV) chloride in toluene.** Thin Solid Films, (2015) **584**, 320-325.

Rowland T, **Hailes HC**, **Evans JRG**, **Sea salt as a potential ocean mirror material.** RSC Advances, (2015) **5**, 38926-38930.

Ruiz-Pérez L, Gaitzsch J, Messager L, **Battaglia G**, Madsen J, Themistou E, Armes SP, **Nanoscale detection of metal-labeled copolymers in patchy polymersomes.** Polymer Chemistry, (2015) 6, 2065-2068

Sadiq SK, **Coveney PV**, **Computing the Role of Near Attack Conformations in an Enzyme-Catalyz**ed Nucleophilic Bimolecular Reaction. Journal of Chemical Theory And Computation, (2014) **11**, 316-324.

Salamat A, Woodhead K, Shah SIU, Hector AL, **McMillan PF**, **Synthesis of USe and UTe type polymorphs of TaN by combining high pressure-temperature pathways with a chemical precursor approach.** Chemical Communications, (2014) **50,** 10041-10044.

Salzmann CG, Murray BJ, Shephard JJ, **Extent of stacking disorder in diamond.** (2015).

Sankar M, Ajithkumar TG, **Sankar G**, Manikandan P. **Supported imidazole as heterogeneous catalyst for the synthesis of cyclic carbonates from epoxides and CO2.** Catalysis Communications, (2015) **59**, 201-205.

Santos VP, Wezendonk TA, Delgado Jaen JJ, Dugulan AI, Nasalevich MA, Islam H-U, Chojecki A, Sartipi S, Sun X, Hakeem AA, Koeken ACJ, Ruitenbeek M, Davidian T, Meima GR, **Sankar G**, Kapteijn F, Makkee M, Gascon J. **Metal organic framework-mediated synthesis of highly active and stable Fischer-Tropsch catalysts.** Nature Communications, (2015) **6**.6451

Sassmannshausen J, Computational studies of the unusual water adduct [Cp2TiMe(OH2)](+): the roles of the solvent and the counterion. Dalton Transactions, (2014) **43**, 11195-11201.

Sathasivam S, Arnepalli RR, Singh KK, Visser RJ, **Blackman CS**, **Carmalt CJ**, **A solution based route to GaAs thin films from As(NMe2)(3) and GaMe3 for solar cells.** RSC Advances, (2015) 11812-11817.

Sathasivam S, Bhachu DS, Lu Y, Bawaked SM, Obaid AY, Al-Thabaiti S, Basahel SN, **Carmalt CJ**, **Parkin IP**, **Highly Photocatalytically Active Iron(III) Titanium Oxide Thin films via Aerosol-Assisted CVD.** Chemical Vapor Deposition, (2015) **21**, 21-25.

Sathasivam S, Bhachu DS, Lu Y, Chadwick N, Althabaiti SA, Alyoubi AO, Basahel SN, **Carmalt CJ**, **Parkin IP**, **Tungsten Doped TiO2 with Enhanced Photocatalytic and Optoelectrical Properties via Aerosol Assisted Chemical Vapor Deposition.** Scientific Reports, (2015) **5**. 10952

Sathasivam S, **Blackman CS**, **Carmalt CJ**, Arnepalli RR, Kumar B, Singh KK, Visser RJ, **Solution processing of GaAs thin films for photovoltaic applications.** Chemistry of Materials, (2014) **26**, 4419-4424.

Sathiwitayakul T, Newton E, **Parkin IP**, Kuznetsov M, Binions R, **Ferrite Materials Produced From Self-Propagating High-Temperature Synthesis for Gas Sensing Applications.** IEEE Sensors Journal, (2015) **15**, 196-200.

Sayer JR, Pesnot T, Campbell F, Koss H, Boyle TP, **Tabor AB**, Walldén K, Buelens F, Waksman G, Gane PJ, Simone M, Selwood DL, **2- and 3-substituted imidazo[1,2-a] pyrazines as inhibitors of bacterial type IV secretion.** Bioorganic and Medicinal Chemistry, (2014) **22**, 6459-6470.

Schauperl M, **Lewis DW, Probing the Structural and Binding Mechanism Heterogeneity of Molecularly Imprinted Polymers.** Journal of Physical Chemistry B, (2015) **119**, 563-571.

Schiller UD, Gompper G, Fleury J-B, Seemann R, **Collective waves in dense and confined microfluidic droplet arrays.** Soft Matter, (2015) **11**, 5850-5861.

Schumacher FF, Nunes JP, Maruani A, **Chudasama V**, Smith ME, Chester KA, **Baker JR**, **Caddick S**, **Next generation maleimides enable the controlled assembly of antibody-drug conjugates via native disulfide bond bridging.** Organic & Biomolecular Chemistry, (2014) **12**, 7261-7269.

Seifert A, Göpfrich K, Burns JR, Fertig N, Keyser UF, **Howorka S**, **Bilayer-spanning DNA nanopores with voltage-switching between open and closed state.** ACS Nano, (2015) **9**, 1117-1126.

Shephard JJ, **Salzmann CG**, **The complex kinetics of the ice VI to ice XV hydrogen ordering phase transition** Chemical Physics Letters, (2015 arXiv:1507.02665

Shephard JJ, Soper AK, Callear SK, Imberti S, Evans JSO, **Salzmann CG**, Polar stacking of molecules in liquid chloroform. Chemical Communications, (2015) **51**, 4770-4773..

Simmance K, van Beek W, **Sankar G**, **Time resolved in situ X-ray diffraction study of crystallisation processes of large pore nanoporous aluminophosphate materials.** Faraday Discussions, (2015) **177**, 237-247.

Smith AM, Perkin S, **Parkes MA**, **Molecular friction mechanisms across nanofilms of a bilayer-forming ionic liquid.** Journal of Physical Chemistry Letters, (2014) **5**, 4032-4037.

Smith MEB, Robinson E, Morais M, Maruani A, Nunes JPM, Caddick S, **Baker JR**, **Chudasama V**, Caspersen MB, Nicholls K, Saxton MJ, **A platform for efficient, thiol-stable conjugation to albumin's native single accessible cysteine.** Organic and Biomolecular Chemistry, (2015) **13**, 7946-7949.

Song J, Huang S, Lu Y, Bu X, Mates JE, Ghosh A, Ganguly R, **Carmalt CJ**, **Parkin IP**, Xu W, Megaridis CM, **Self-Driven One-Step Oil Removal from Oil Spill on Water via Selective-Wettability Steel Mesh.** ACS Applied Materials & Interfaces, (2014) **6**, 19858-19865.

Sotelo-Vazquez C, Noor N, Kafizas A, Quesada-Cabrera R, **Parkin IP**, Durrant JR, Scanlon DO, Taylor A, **Multifunctional P-doped TiO2 Films: A new approach to self-cleaning, transparent conducting oxide materials.** Chemistry of Materials, (2015) **27**, 3234-3242.

PUBLICATIONS

Sprick RS, Jiang J-X, Bonillo B, Ren S, Ratvijitvech T, Guiglion P, **Zwijnenburg MA**, Adams DJ, Cooper AI, **Tunable Organic Photocatalysts for Visible-Light-Driven Hydrogen Evolution.** Journal of The American Chemical Society, (2015) **137**, 3265-3270.

Stewart HM, Shevlin SA, **Catlow CRA**, **Guo ZX**, **Compressive Straining of Bilayer Phosphorene Leads to Extraordinary Electron Mobility at a New Conduction Band Edge**. Nano Letters, (2015) **15,** 2006-2010.

Stratford SA, Arhangelskis M, **Bučar D-K**, Jones W, **Solid-state photoreactivity of 9-substituted** acridizinium **bromide salts.** CrystEngComm, (2014) **16**, 10830-10836.

Suter JL, Groen D, **Coveney PV**, **Chemically specific multiscale modeling of clay-polymer nanocomposites reveals intercalation dynamics, tactoid self-assembly and emergent materials properties.** Advanced Materials, (2015) **27**, 966-984.

Suter JL, Groen D, **Coveney PV**, **Clay-polymer nanocomposites: chemically specific multiscale modeling of clay-polymer nanocomposites reveals intercalation dynamics, tactoid self-assembly and emergent materials properties.** Advanced Materials, (2015) **27**.10.1002/adma.201570034

Swadling JB, Wright DW, Suter JL, **Coveney PV**, **Structure, dynamics, and function of the hammerhead ribozyme in bulk water and at a clay mineral surface from replica exchange molecular dynamics.** Langmuir: the ACS journal of surfaces and colloids, (2015) **31**, 2493-2501.

Tafreshi SS, **Roldan A**, **de Leeuw NH**, **Density Functional Theory Study of the Adsorption of Hydrazine on the Perfect and Defective Copper (100), (110), and (111) Surfaces.** Journal of Physical Chemistry C, (2014) **118,** 26103-26114.

Tafreshi SS, **Roldan A**, **de Leeuw NH**, **Hydrazine network on Cu(111) surface: A Density Functional Theory approach.** Surface Science, (2015) **637**, 140-148.

Tilocca A, **Atomic-scale models of early-stage alkali depletion and SiO2-rich gel formation in bioactive glasses**. Physical Chemistry Chemical Physics, (2015) **17**, 2696-2702.

Tobaldi DM, Pullar RC, Seabra MP, Labrincha JA, Gualtieri AF, Belen Jorge A, **McMillan PF**, Binions R, **Influence of sol counter-ions on the anatase-to-rutile phase transformation and microstructure of nanocrystalline TiO.** CrystEngComm, (2015) **17**, 1813-1825.

Travis W, Gadipelli S, **Guo Z**, **Superior CO2 adsorption from waste coffee ground derived carbons.** RSC Advances, (2015) **5**, 29558-29562.

Uzoh OG, Galek PTA, **Price SL**, **Analysis of the conformational profiles of fenamates shows route towards novel, higher accuracy, force-fields for pharmaceuticals.** Physical Chemistry Chemical Physics, (2015) **17**, 7936-7948.

Varley TS, Rosillo-Lopez M, Sehmi S, Hollingsworth N, **Holt KB**, **Surface redox chemistry and mechanochemistry of insulating polystyrene nanospheres.** Physical Chemistry Chemical Physics, (2015) **17**, 1837-1846.

Vasheghani Farahani SK, Mudd JJ, McConville CF, Veal TD, **Scanlon DO**, Watson GW, Bierwagen O, White ME, Speck JS, **Valence-band density of states and surface electron accumulation in epitaxial SnO2 films.** Physical Review B - Condensed Matter and Materials Physics, (2014) **90**. 155413

Villa A, Campisi S, Mohammed KMH, **Dimitratos N**, Vindigni F, Manzoli M, Jones W, Bowker M, Hutchings GJ, Prati L, **Tailoring the selectivity of glycerol oxidation by tuning the acid-base properties of Au catalysts.** Catalysis Science & Technology, (2015) **5**, 1126-1132.

Villa A, Chan-Thaw CE, Prati L, Dimitratos N, Hammond C, Hutchings GJ, **Glycerol oxidation using gold-containing catalysts.** Accounts of Chemical Research, (2015) **48**, 1403-1412.

Viswanathan P, Johnson DW, Cameron NR, Hurley C, **Battaglia G**, **3D surface functionalization of emulsion-templated polymeric foams.** Macromolecules, (2014) **47**, 7091-7098.

Viswanathan P, Ondeck MG, Engler AJ, Chirasatitsin S, Ngamkham K, **Battaglia G**, Reilly GC, **3D surface topology guides stem cell adhesion and differentiation.** Biomaterials, (2015) **52**, 140-147.

Viswanathan P, Themistou E, Ngamkham K, Reilly GC, Armes SP, **Battaglia G**, **Controlling Surface Topology and Functionality of Electrospun Fibers on the Nanoscale using Amphiphilic Block Copolymers To Direct Mesenchymal Progenitor Cell Adhesion.** Biomacromolecules, (2014) **16**, 66-75.

Volpe G, Gigan S, **Optical manipulation with random light fields: From fundamental physics to applications.** Optical Trapping Applications, (2015). doi:10.1364/OTA.2015.OtW2D.1

Walsh A, **Scanlon DO**, Chen S, Gong XG, Wei S-H, **Self-regulation mechanism for charged point defects in hybrid halide perovskites.** Angewandte Chemie - International Edition, (2015) **54**, 1791-1794.

Wang L, Yuan P-F, Wang F, Sun Q, Liang E-J, Jia Y, **Guo Z-X**, **First-principles investigation of negative thermal expansion in II-VI semiconductors.** Materials Chemistry and Physics, (2014) **148**, 214-222.

Wang SY, Soe MT, Guo KT, Zhang XL, **Guo ZX**, **An effective template-free synthesis strategy for hierarchical titanium oxide hybrids: Tailoring the solvent environment.** RSC Advances, (2015) **5**, 41059-41065.

Wang X, Kafizas A, Li X, Moniz SJA, Reardon PJT, Tang J, **Parkin IP**, Durrant JR, **Transient Absorption Spectroscopy of Anatase and Rutile: The Impact of Morphology and Phase on Photocatalytic Activity.** Journal of Physical Chemistry C, (2015) **119**, 10439-10447.

Wang Z, Lambden S, Nandi M, Tomlinson J, Dyson A, Taylor V, Sujkovic E, McDonald N, **Caddick S**, Singer M, Leiper J, **A novel dimethylarginine dimethylaminohydrolase (DDAH-1) inhibitor improves survival, hemodynamics and organ function in rodent sepsis.** Nitric Oxide-Biology and Chemistry, (2014) **42**, 100.

Wang Z-Y, Wang F, Sun Q, **Guo Z-X**, Jia Y, Wang X-Q, Zhou Y-L, **Effects of in-plane stiffness and charge transfer on thermal expansion of monolayer transition metal dichalcogenide.** Chinese Physics B, (2015) **24**. 026501

Whiting GT, Kondrat SA, Hammond C, **Dimitratos N**, Morgan DJ, Dummer NF, Bartley JK, Taylor SH, Hutchings GJ, He Q, Kiely CJ, **Methyl formate formation from methanol oxidation using supported gold-palladium nanoparticles.** ACS Catalysis, (2015) **5**, 637-644.

Wilding MC, Wilson M, **McMillan PF**, Benmore CJ, Weber JKR, Deschamps T, Champagnon B, **Structural properties of YO-AlO liquids and glasses: An overview. Journal of Non-Crystalline Solids**, (2015) **407**, 228-234.

Wilding MC, Wilson M, **McMillan PF**, Deschamps T, Champagnon B, **Low frequency vibrational dynamics and polyamorphism in YO-AlOglasses.** Physical Chemistry Chemical Physics, (2014) **16,** 22083-22096.

Wills AS, **Validation of magnetic structures**. Z kristallogr, (2015) 53,58

Wilson SS, Bosco JP, Tolstova Y, Atwater HA, **Scanlon DO**, Watson GW, **Interface stoichiometry control to improve device voltage and modify band alignment in ZnO/CuO heterojunction solar cells.** Energy and Environmental Science, (2014) **7**, 3606-3610.

Wobbe MCC, Kerridge A, **Zwijnenburg MA**, **Optical excitation of MgO nanoparticles; a computational perspective.** Physical Chemistry Chemical Physics, (2014) **16**, 22052-22061.

Woodley SM, Catlow CR, **High performance computing in the chemistry of materials.** Physical Chemistry Chemical Physics, (2014) **16**, 21001.

Wu M-Y, Wang L, Jia Y, Sun Q, **Guo Z-X**, **Theoretical study of hydration in YMoO: Effects on structure and negative thermal expansion.** AIP Advances, (2015) **5**.027126

Yim CM, Pang CL, Hermoso DR, Dover CM, Muryn CA, Maccherozzi F, Dhesi SS, Pérez R, **Thornton G**, **Influence of support morphology on the bonding of molecules to nanoparticles.** Proceedings of the National Academy of Sciences, (2015) **112**, 7903-7908.

Yim CM, Pang CL, **Thornton G**, **Probing the local electronic structure of the cross-linked (1×2) reconstruction of rutile TiO2(110).** Surface Science, (2015). doi:10.1016/j.susc.2015.04.022

Yuan P-F, Sun Q, Jia Y, **Guo ZX**, **Role of charge transfer in dehydrogenation of M(NHBH) (M = Mg, Sr).** Journal of Physical Chemistry C, (2014) **118**, 18315-18324.

Zanni M, Jemmis ED, Aravamudhan S, Pallipurath A, Arunan E, Schnedermann C, Mishra AK, Warren M, Hirst JD, John F, Pal R, Helliwell JR, Moirangthem K, Chakraborty S, Dijkstra AG, Chowdhury PR, Ghiggino K, Miller RJD, Meech S, Medhi H, Hariharan M, Ariese F, Edwards A, Mallia AR, Umapathy S, Nielsen MM, Hunt N, Tian Z-Y, Skelton J, **Sankar G**, Goswami D, **Time and Space resolved Methods: general discussion.** Faraday Discussions, (2015) **177**, 263-292.

Zeinalipour-Yazdi CD, Willock DJ, Thomas L, Wilson K, Lee AF, **CO adsorption over Pd nanoparticles: A general framework for IR simulations on nanoparticles.** Surface Science, (2015). doi:10.1016/j.susc.2015.07.014

Zenonos C, **Lewis DW, Sankar G**, **Location and orientation of the N,N-diisopropylethylamine template molecule in the AlPO4-18 framework by X-ray synchrotron diffraction and molecular modelling.** Chinese Journal of Catalysis, (2015) **36**, 874-879.

Zhang S, Li C, **Guo ZX**, Cho J-H, Jia Y, Su W-S, **Magnetic evolution and anomalous Wilson transition in diagonal phosphorene nanoribbons driven by strain.** Nanotechnology, (2015) **26**.295402

Zhu B, Qiu K, **Guo Z**, Shang C, **Naturally derived porous carbon with selective metal- and/or nitrogen-doping for efficient CO2 capture and oxygen reduction.** Journal of Materials Chemistry A, (2015) **3**, 5212-5222.

Wolthers, Mariette VH, Towards a stable astronomical time scale for the Paleocene: Aligning Shatsky Rise with the Zumaia – Walvis Ridge ODP Site 1262 composite. Newsletters on Stratigraphy, (2015). **48** 91-110

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