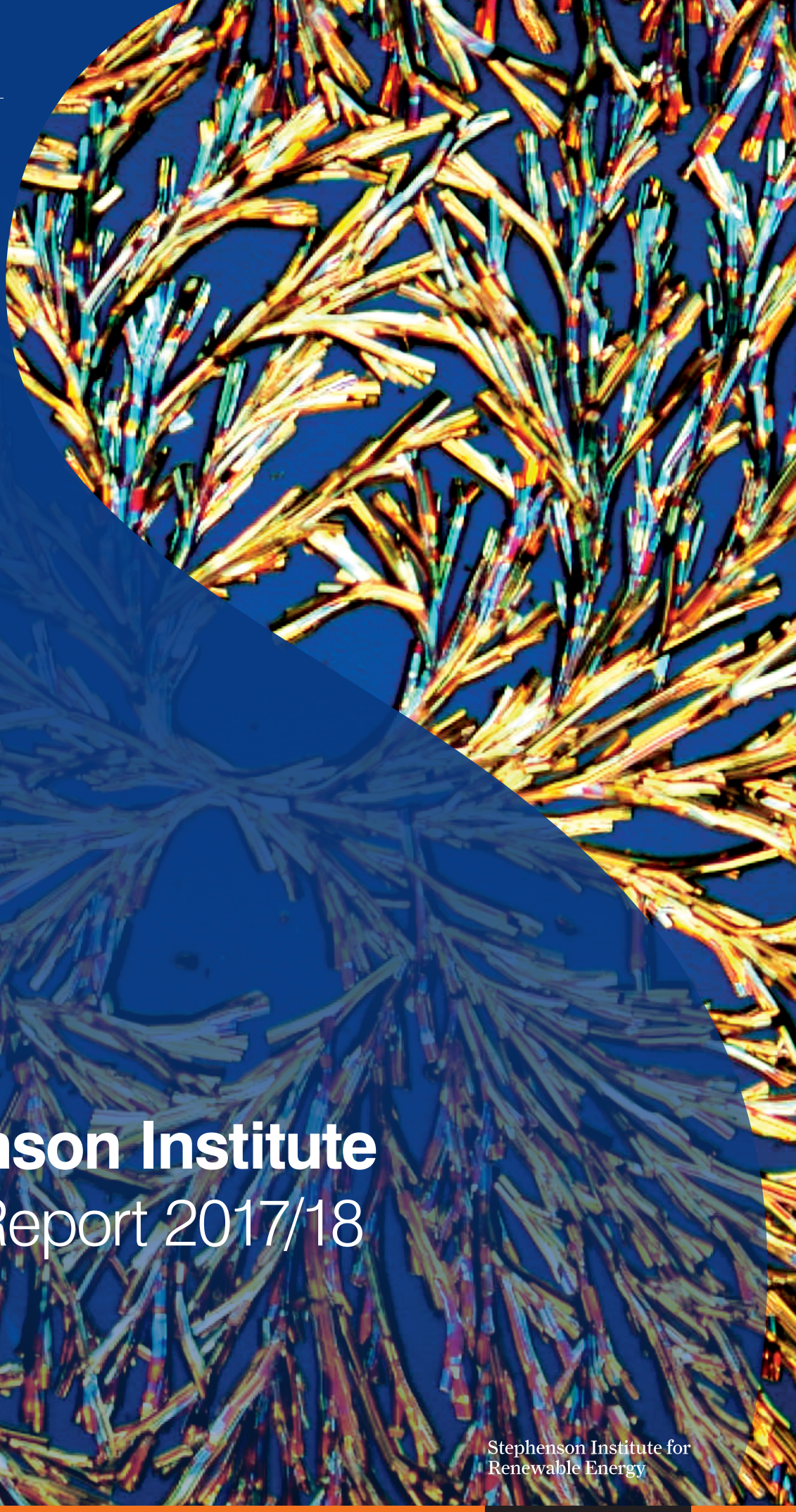
UNIVERSITY OF LIVERPOOL



Stephenson Institute
Annual Report 2017/18

Stephenson Institute for Renewable Energy

LIFE CHANGING
World Shaping

The Stephenson Institute for Renewable Energy

Contents

Front cover image: Optical microscopy of antimony selenide crystals. Denser, void-free material grown using slightly different conditions is used for solar cells (Dr Laurie Phillips)

Director's Welcome

Welcome to the SIRE Report for 2017/18 – a snapshot of our work on the chemistry and physics of energy storage, conversion, efficiency, and sustainability.

Our aim is to work on topics that transform energy futures through fundamental science, understanding and controlling interfaces, new materials, and devices. We complement the large number of research groups and institutes that concentrate on engineering aspects of energy with our unique focus on the physical sciences for energy research.

I would like to thank Prof Ken Durose for heading the Institute between 2014 and 2017 during the establishment and development of our new research laboratories in the Chadwick building. I look forward to leading SIRE as the new Director. For me, the most rewarding moments of my research career have been discoveries that arise when working across disciplines. This is the essence of SIRE.

2017/18 was an excellent time for staff in SIRE. Congratulations are in order for four staff who were promoted in 2017: In Physics, Professor Tim Veal to a personal chair for his work on materials physics of semiconductors, Dr Jon Alaria to Senior Lecturer for his work on materials design and thermoelectrics and Dr Frank Jäckel to Senior Lecturer for his work on nanomaterials and photocatalysis. In Chemistry, Dr Alex Cowan was promoted to Reader for his work in electro- and photo-catalytic conversion. Congratulations to a further two staff for their promotions in 2018: In Physics, Professor Vin Dhanak to a personal chair for his work on X-ray photoelectron spectroscopy and, in Chemistry, Dr Frédéric Blanc to Reader for his work on solid state nuclear magnetic resonance, for which he was awarded the Institute of Physics and Royal Society of Chemistry RSC Annual Prize for Excellent Contribution in Magnetic Resonance. You can read more about their work in the research sections of this brochure.

As the Institute matures, it has been another bumper period for PhD graduations. Seventeen of our early stage research colleagues successfully defended their theses in 2017: Arturas Adomkevicius, Liz Cocklin, Nor Azam Bin Endot, Marta Fernández Giménez, Mark Forster, Tom Galloway, Michael Graham, Jon Lee, Gaia Neri, Nadiah Mohamad Noh, Lorena Martin Olivera, Georgios Papageorgiou, Annette Pressman, Aldo Reyes, Chris Sole, Ebenezer Tetsi, Tom Whittles – their thesis titles and photos appear towards the end of this report. Everyone in the team congratulates all of them and wishes them all well in their future careers! Many more PhD students successfully completed and defended their thesis in 2018 and they will be featured in our next report.

Thank you for reading our annual report. I do hope that if you wish to know more or to collaborate with us you will feel welcome to get in touch with any of the Institute's experts using the directory of expertise at the back of this report.

Laurence Hardwick,
Director, SIRE

Impact and Events

EPSRC Centre for Doctoral Training in New and Sustainable Photovoltaics – CDT-PV: Summer School, Showcase Event and Cohort Training

The Centre for Doctoral Training in New and Sustainable Photovoltaics (CDT-PV) is a UK national centre having the mission of training future leaders for research and industry in solar energy generation. This is necessary if the UK is to take its place in the revolution in energy provision – focussing more and more on renewable resources. Our central theme is that the next generation of solar photovoltaic panels will be able to satisfy the needs of both the mass market and for special products such as hand held and indoor electronic devices. These solar cells will need to be made from the new and sustainable materials that are the focus of our research and training.

Led from Liverpool, CDT-PV comprises seven academic teams giving both a critical mass and complete coverage of the research themes and training needs relevant to the future of solar energy generation. The partners and their expertise are: University of Liverpool, Thin film solar energy materials and devices; University of Bath, Modelling of PV devices and novel inorganic materials for PV; University of Cambridge, Organic PV; University of Loughborough, PV systems and performance; University of Oxford, Perovskite materials and devices; University of Sheffield, Processing for organic and perovskite PV materials; and University of Southampton, Silicon and nanotechnology.

It is a principle of all CDTs that the PhD students play an important part in deciding what training and development they need, and which should be provided as part of the CDT experience. The 2017 academic year got off to an exceptional start with a student-led Summer School held in Uppsala, Sweden in June. There was a comprehensive programme held over two days with talks from Alex Castro, on IKEA's sustainability plan; from Annika Skoglund, University of Uppsala on '*Environmental activism in large energy companies*'; an industrial perspective on CIGS from Eric Jaremalm, Midsummer; and technical talks on perovskites, CZTS and artificial photosynthesis, from Gerrit Boschloo, Charlotte Platzer Björkman and Haining Tian, all from Uppsala University. Our students took the opportunity to share their own technical presentations and self-taught classes on research methods and preparation of papers.

The 2017 academic year got off to an exceptional start with a student-led Summer School held in Uppsala, Sweden in June.

Above: 2017 CDT-PV Showcase organisers – Tom Shalvey, Jonathan Warby, Rachel Greenhalgh and Joel Smith.

2017 saw CDT-PV joined by its fourth cohort of 11 new PhD students from backgrounds including physics, chemistry, mathematics and engineering. This marked the start of the annual cycle of training, with the students coming to Liverpool for the first module of seven, 'Fundamentals of Photovoltaics'.

We were delighted to be joined by colleagues from industry: Prof Paul Warren, visiting Professor of Physics at the University of Liverpool gave an overview of the coated glass industry – NSG/Pilkington are the world's largest supplier of glass to the thin film PV industry. Dr Eric Don gave insight into SMEs with examples from his own career and how it led to his starting Semimetrics Ltd, a company supplying advanced measurement equipment for research and semiconductor metrology needs. We were also joined by one of the CDT's International Advisory Panel members, Dr Phil Dale from the University of Luxembourg. He commented that the student talks were above national standard and highlight the level of research output from the CDT. Our student-judged award for the Best Talk went to Nicola Courtier from Southampton for her work on drift-diffusion modelling in perovskite solar cells. The fortnight concluded with the annual CDT Showcase event, this time in the Royal Liver Building on the Liverpool waterfront, and which was attended by over 100 scientists.

October 2018 saw us welcome our final cohort of 14 students, bringing the total to 50 plus 12 leavers. Those finishing their PhDs this year will be our first graduates, and we wish them all the best in their future careers.

Further into the academic year, the fourth cohort of students continued their gruelling cycle of training, with two-week courses in each of the seven different university partner cities.

Their stay in Sheffield saw them learning about advanced polymer characterisation tools, laboratory research methods, and they visited the SME Ossila Ltd who supply specialist materials and know-how to solar PV research laboratories. At the weekend they took some well-deserved time off with a trip to the Peak District, as you can see from the photograph.

The CDT's training continues beyond the first-year core events, and this year the students requested some special training sessions on research ethics, unconscious bias, and a workshop on topics relevant to final year PhD studies. Since our first cohort of 12 students were writing their PhD theses in preparation for examination in the autumn, a workshop held in London in March 2018 was focussed on writing skills, CV preparation and some presentations from people working outside of the university environment including with large companies and start-ups.

This year the CDT was also fortunate to be joined by our new Academic Manager, Dr Asim Mumtaz. Asim joined us from University of Warwick after formerly studying at Durham and Cambridge and working both in the UK and the USA.

Ken Durose, Director CDT-PV

Above: CDT-PV's fourth cohort taking some time to relax in the Peak District during the Sheffield module.

The ECS Northwest Student Chapter Conference, Liverpool UK June 8, 2017

On June 8 2017 Nikolas Antonatos and Lisa Rhodes-Martin, chair and vice-chair of the Electrochemical Society UK Northwest Student Chapter organised a student-led conference in the Stephenson Institute.

The conference saw over 40 students and academics from the Universities of Liverpool, Manchester and Lancaster coming together to share knowledge and ideas about all things electrochemistry.

Guest speaker Prof. Charles Monroe from The University of Oxford gave a talk entitled: '*Modelling lithium/oxygen cells to rationalize experimental performance*', which gave an insight into how both theoretical and practical efforts are used to elucidate design factors that control the rate capability and capacity of Li/O_2 batteries. The talk was very informative and the chapter hopes to welcome Charles back in the future to give more talks on his research field.

The conference also included a series of talks given by our student members: Tom Galloway from University of Liverpool (UoL) gave a talk on an Enhanced Raman Technique using Isolated Shell Nanoparticles, José Antonio Coca Clemente from UoL presented on Mixed Metal Layered Transition Metal Oxides, Craig Armstrong from Lancaster University presented on Cobalt Complexes for Non-aqueous Redox-flow Batteries, Samuel Booth from University of Manchester presented on Metal Deposition at a Liquid/Liquid Interface, Charlotte Smith from UoL presented on Conjugated Microporous Polymers and finally Manesh Mistry presented on DFT studies at Electrode Electrolyte interfaces. All of our student talks were very interesting and gave us the opportunity to experience and appreciate each other's research and helped strengthen the research ties between our North Western institutes.

From left to right: Charlotte Smith, Laura Cabo-Fernandez, Scott Lewis, Laurence Hardwick, Tom Galloway, Filipe Braga Nogueira, Lena Reichenbach, José Coca Clemente, Gaia Neri, Stefano Mensa, Vivek Padmanabhan.

The event also included a Poster session and was concluded with an award ceremony where sponsors *Alvatek* and *Blue Scientific* presented awards for best talk and best poster. This year's prize winners were Craig Armstrong from Lancaster University and Gaia Neri from UoL.

Nanochemical systems for energy efficient maritime transport

The marine transport industry accounts for 1,000 million tonnes of CO_2 emissions each year and emissions are predicted to increase around 250% by 2050. Researchers at the Stephenson Institute are mitigating the ecological and economical costs by using eco-friendly nanochemicals that keep ship hulls cleaner and more hydrodynamic for better fuel efficiency.

The challenge

The accumulation of microorganisms, plants and small animals on wet surfaces, a natural but undesirable phenomenon known as biofouling, increases shipping fuel consumption and CO_2 emissions by up to 40%.

Work led by Professor Dmitry Shchukin has delivered an environmentally friendly, cost-efficient class of antifouling materials. It has the potential to greatly reduce CO_2 emissions in this vital transport sector, which are projected to reach 17% of global CO_2 production by 2050.

Research action

Shchukin's group have developed an innovative and careful design to control nanocapsules that release the antifouling agent on demand over years, preventing the need for regular manual hull cleaning and reducing maintenance costs. It can also be painted onto existing ships, massively increasing real-world use and environmental benefits.

Working in partnerships

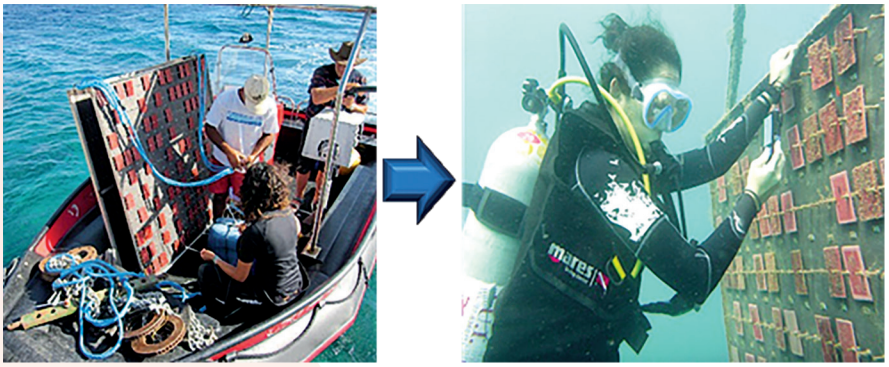
Working within a large EU consortium of 19 academic partners and companies called the Byefouling programme, the Stephenson Institute for Renewable Energy team have rapidly translated their fundamental advances into practical application in the paints industry. Closely interacting academic and industrial teams have ensured a focus on developing a product fit for purpose in the stern tests of the world's oceans.

Outputs and outcomes

The products designed by Shchukin's group are currently undergoing field trials to test antifouling activity on industrial shipping fleets. Biofouling causes significant problems in other major industry sectors including aquaculture, wind farms and offshore oil industries. The new antifouling agents can also reduce operational expenses caused by microorganism on underwater platforms, pipelines and sea-farms.

Nanocapsule technology has delivered an environmentally friendly, cost-efficient class of antifouling materials that can significantly reduce CO_2 emissions in shipping and allied industries.

Below: Immersed floating structure in Eilat (northern Red Sea) with the experimental panels at the day of deployment and during the underwater photographs.



NANOCHEMICAL SYSTEMS FOR ENERGY EFFICIENT MARITIME TRANSPORT:

1,000

The marine transport industry accounts for 1,000 million tonnes of CO_2 emissions each year

Working within a large EU consortium of 19 academic partners and companies

2050

This transport sector is projected to reach 17% of global CO_2 production by 2050

250%

Marine transport CO_2 is predicted to increase around 250% by 2050.

40%

Biofouling increases shipping fuel consumption and CO_2 emissions by up to 40%.

Nanocapsule technology has delivered an environmentally friendly, cost-efficient solution

Launch of SEAFUEL: the European project for sustainable integration of renewable fuels in local transportation

The official kick-off meeting of the SEAFUEL project was held in Galway, Ireland, on January 25th and 26th 2018.

With a total budget of €3,497,632 and for 3 years, the SEAFUEL projects aims to use the renewable resources across the Atlantic Area to power the local transport fleet and support the shift towards a low-carbon economy. The project will use the expertise and infrastructure of the partners in renewable energy, namely solar, wind and marine, to demonstrate the viability of hydrogen as a fuel to be used by the local transport authorities.

Among the first activities of the project was the celebration of the first transnational meeting of partners that took place on January 25th and 26th at the facilities of the National University of Ireland (NUI Galway), which leads the project. The kick-off meeting provided the perfect opportunity for all partners to review the project objectives and the work plan, with a short overview on each project activity foreseen in phase 1. Furthermore, on January 26th a session was held with external experts from the Big Hit and GenComm projects, the second one funded by INTERREG NWE, with the intention of establishing communication bridges with other complementary hydrogen projects from the beginning of the project.

The aim of SEAFUEL is to demonstrate the feasibility to power local transportation networks using fuels produced by renewable energies and seawater, with no net carbon footprint as promoted by the resource-efficient flagship initiative COM(2010)2020. It will cover technical innovation by a demonstration plant, a framework for policy implementation and a sustainability analysis of production, distribution and usage of hydrogen as an alternative fuel in remote Atlantic regions. SEAFUEL proposes a sustainable way to power local transportation in isolated regions using renewable resources such as sun, wind and seawater.

SEAFUEL will focus on enhancing the green growth and blue economy and paving the grounds for common renewable energy policies to promote clean and sustainable transport systems. Isolated areas such as islands face the specific challenge of the high cost of electricity and fuel and their dependency on mainland infrastructures. SEAFUEL will target these regions where 30% of fuel consumption comes from local transportation. The project will drastically reduce greenhouse emissions, particulate matter and NO_2 in line with the Clean Air programme 2008/50/EC, and provide a pathway for isolated regions to become energetically independent, leading to future installations in the other Atlantic regions. An alternative fuels model for islands will be developed to fulfil the requirements of the Partners' Regional Innovation Strategies (RIS3) aimed at low carbon economy and efficient use of marine resources.

The SEAFUEL project is co-financed by the 2014-2020 INTERREG Atlantic Area programme (http://www.atlanticarea.eu/) that supports transnational cooperation projects in 36 Atlantic regions of five countries: France, Ireland, Portugal, Spain and the United Kingdom, contributing to the achievement of economic, social and territorial cohesion. The partners of the project are: from Ireland, the National University of Ireland Galway and Comharchumann Fuinnimh Oileáin Árann Teoranta; from the United Kingdom, the University of Liverpool (Dr Alex Cowan of SIRE), Action Renewables, HyEnergy Consultancy Limited and Logan Energy; from Spain, the Institute of Technology and Renewable Energies of Tenerife and the Tenerife Energy Agency; The Regional Agency for Energy and Environment of the Autonomous Region of Madeira (Portugal) and the European Hydrogen Association (Belgium).

THE SEAFUEL PROJECT:

€3,497,632 Budget for 3 years

JAN

The first transnational meeting of partners took place on January 25th and 26th

30%

SEAFUEL will target regions where 30% of fuel consumption comes from local transportation

36 The INTERREG Atlantic Area programme supports transnational cooperation projects in 36 Atlantic regions of five countries.

SEAFUEL proposes a sustainable way to power local transportation in isolated regions using renewable resources such as sun, wind and seawater.

SIRE Seminar Series 2017/18

All staff in SIRE would like thank the seminar speakers for 2017/18. Our seminars are open to all. Details of the current programme are at www.liverpool.ac.uk/renewable-energy/events/

Date	Name	Affiliation	Title
Monday 20 March 2017	Professor Nikolai Gaponik	Physical Chemistry, Technical University Dresden	Quantum Dots in ionic salt matrices: robust composites for optoelectronics and photonics
Friday 30 June 2017	Dr Graham Ball	School of Chemistry, University of New South Wales	Characterization of alkane sigma-complexes and related exotica using NMR spectroscopy
Thursday 13 July 2017	Dr Kent Griffith	Department of Chemistry, University of Cambridge	Energy Storage Mechanisms and Structural Characterisation of Mixed-metal Complex Oxides
Thursday 7 September 2017	Prof Jian-Feng Li	College of Chemistry, Xiamen University, China	Plasmon-enhanced Raman/fluorescence spectroscopy using shell-isolated mode
Tuesday 31 October 2017	Dr Rob Palgrave	Department of Chemistry, University College London	Photoemission spectroscopy as an analytical technique applied to energy materials
Tuesday 14 November 2017	Dr Emma Kendrick	Warwick Manufacturing Group, University of Warwick	Sodium ion batteries: materials to devices
Tuesday 28 November 2017	Prof Julie McPherson	Department of Chemistry, University of Warwick	Electrocatalytic applications of conducting diamond membrane electrodes
Tuesday 5 December 2017	Dr Cristina Tealdi	Department of Chemistry, University of Patvia, Italy	Ionic conductors for clean energy applications: tailoring their properties through defects and strain
Tuesday 12 December 2017	Charlotte Smith	Department of Chemistry and SIRE, University of Liverpool	Conjugated microporous polymers for the support of CO_2 reduction
Tuesday 20 February 2018	Ken Inglis	Department of Chemistry and SIRE, University of Liverpool	Solid-State NMR Investigation of $La_3Li_3W_2O_{12}$: A Perovskite with Lithium on both A- and B-Sites
Friday 23 February 2018	Dr Georgios Tritsaris	Deregallera Ltd.	Electronic structure theory and simulation of complex surfaces and interfaces for energy
Wednesday 28 March 2018	Dr Dmitry Volodkin	Department of Chemistry, Nottingham Trent University	Encapsulation of fragile biomolecules through mesoporous $CaCO_3$ crystals
Tuesday 10 April 2018	Lisa Rhodes-Martin	Department of Physics and SIRE, University of Liverpool	Structural and electrochemical characterisation of ionic liquids
Tuesday 17 April 2018	Prof David Fermin	Department of Chemistry, University of Bristol	Electrocatalysis at Metallic and Highly Correlated Electron Phases: Worlds Apart
Thursday 14 June 2018	Prof Ulrich Stimming	Dept. of Chemistry, University of Newcastle	Molecular Processes in Li- and Na-Ion and Redox Flow Batteries

Research Group Expertise and Highlights

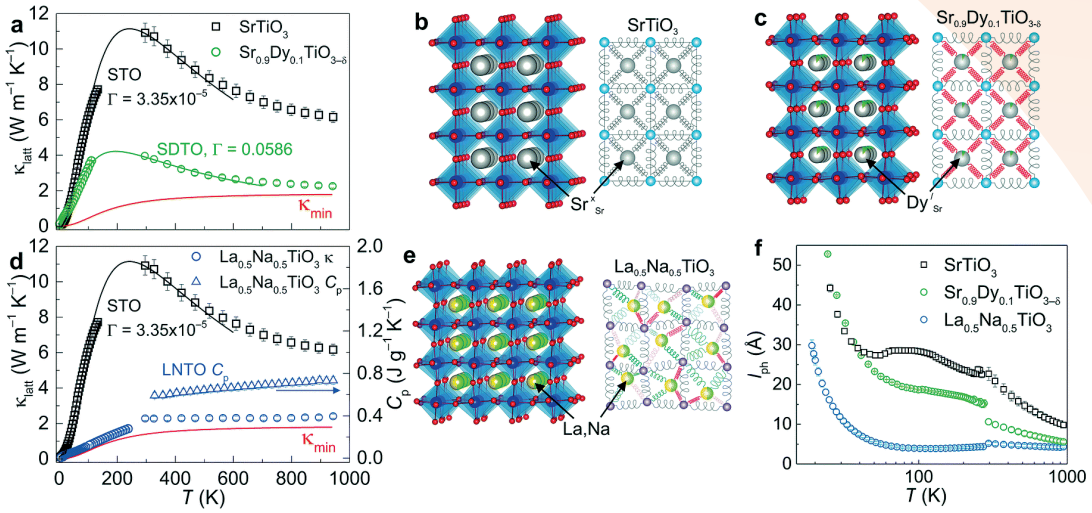
Crystal growth, Magnetism and Thermoelectrics

Jonathan Alaria

We specialise in single crystal bulk growth, thin film growth by pulsed laser deposition and physical characterisation. High quality crystals are an essential part of our research, enabling us to determine fundamental properties of new or previously misunderstood materials. Physics understanding and methodologies (such as quantum oscillations) are combined with chemistry know-how and intuition. In terms of renewable energy research, the main focus is the design of novel ways to break the conventional interdependence of thermal and electronic conductivity in order to develop improved thermoelectric materials.

Highlight: Phonon-glass electron-crystal behaviour by A site disorder in n-type thermoelectric oxides

Oxide materials are of current interest as high-temperature energy-harvesting thermoelectrics in the automotive and manufacturing sectors due to their low cost, low toxicity and high chemical robustness. The phonon-glass electron crystal (PGEC) concept which has been successfully used to optimise the thermoelectric figure of merit (ZT) in clathrates and skutterudites by combining the high electronic conduction of a crystal with the low thermal conduction of a glass is an approach which has not yet been realised in oxides due to the strong coupling between electronic and thermal transport. Through crystal chemistry engineering of the ABO_3 perovskite based around a combined experimental and computational understanding of the mechanisms responsible, PGEC behaviour has been achieved for the first time in oxide thermoelectrics by decoupling thermal and electronic transport.

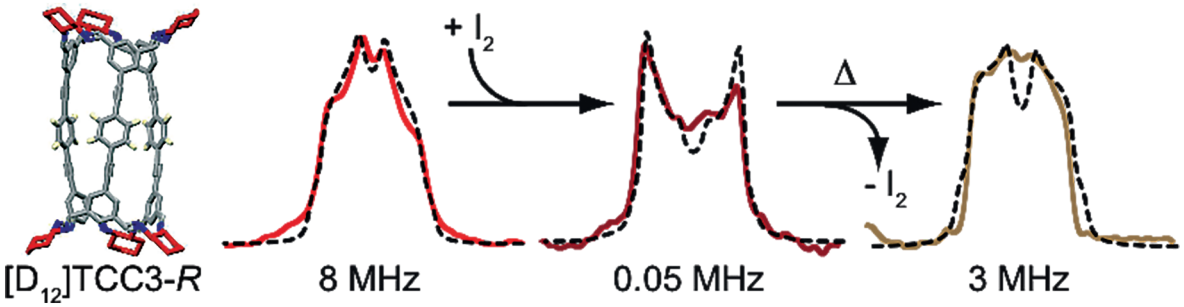


Measured κ_{latt} for phonon-crystals $SrTiO_3$ and $Sr_{0.9}Dy_{0.1}TiO_{3-\delta}$ are shown in (a) and are compared against the Debye-Callaway model for crystalline solids (solid lines), alongside example spring models (b) and (c), illustrating phonon coupling between nearest-neighbours in the crystal structure with identical force constants. The theoretical κ_{min} of STO is calculated from Cahill's model for disordered crystalline solids, and is compared against the experimental data in (a) and (d). The κ_{latt} of $La_{0.5}Na_{0.5}TiO_3$ (LNTO) shown in (d) cannot be modelled as a phonon-crystal using the Callaway model, and compares much more closely to κ_{min} of a phonon-glass, with a temperature dependence that follows the contribution of the heat capacity (C_p) shown on the right-hand axis of (d). The vibrational disorder of LNTO resulting from phonon interactions between randomly distributed A site cations with high mass contrast and the rest of the structure is illustrated through the spring model in (e). Phonon mean free paths shown in (f) are extracted using the measured κ_{latt}, C_p, and speed of sound v_s. Reproduced with permission. Copyright Royal Society of Chemistry 2017.

L. M. Daniels, S. N. Savvin, M. J. Pitcher, M. S. Dyer, J. B. Claridge, S. Ling, B. Slater, F. Corà, J. Alaria, and M. J. Rosseinsky, Phonon-glass electron-crystal behaviour by A site disorder in n-type thermoelectric oxides, Energy Environ. Sci. **10** (2017) 1917-1922.

Exploiting Magnetic Resonance in Materials Chemistry

Frédéric Blanc



Magnetic resonance spectroscopy enables advances in the understanding of the structure, dynamics and behaviour of a large range of chemical systems to be obtained. We exploit the atomic resolution sensitivity of magnetic resonance to probe the mobility of lithium and oxide ions in electrolytes materials for application in energy storage and conversion devices, to follow the dynamics of supramolecular assemblies with molecular capture and release properties and to identify catalytic intermediates in heterogeneous catalysts as well as their host guest interactions. Recent research highlights also include the development of hyperpolarisation magnetic techniques to detect the nuclear spins of extremely insensitive nuclei. Frederic Blanc and colleagues in the University's Faculty of Science and Engineering and its Faculty of Health and Life Sciences have been awarded £1.3 million in 2018 from the Engineering and Physical Sciences Research Council (EPSRC) to enhance the University's capabilities in very high field 800 MHz Nuclear Magnetic Resonance (NMR). The upgrade will convert an existing solution-state system (see picture) to a NMR spectrometer with dual solution-solid state capabilities, thereby strategically differentiating the Liverpool system from other very high field spectrometers in the UK.

Highlight: Ultra-Fast Molecular Rotors within Porous Organic Cages

In collaboration with colleagues at the Materials Innovation Factory at the University of Liverpool, we have discovered that a particular class of supramolecular assemblies can act as molecular capture and release materials by application of an external stimulus (for example, temperature). Using variable temperature NMR spectra, we show that two different porous organic cages with tubular architectures are ultra-fast molecular rotors. The central unit rings that frame the "windows" to the cage voids display very rapid rotational rates with low activation energy barriers. These cages behave as hosts to iodine guest molecules, which dramatically slows down the rotational rates of the "windows", demonstrating potential use as smart materials. Recent research highlights also include the development of hyperpolarisation magnetic techniques to detect the nuclear spins of extremely insensitive nuclei.

Example of an ultra-fast molecular rotors within a porous organic cage and associated deuterium NMR spectra upon adsorption and release of iodine guest molecule. Published under a Creative Commons Attribution License in Chem. Eur. J. 23, 1-6 (2017).

A. R. Hughes, N. J. Brownbill, R. C. Lalek, M. E. Briggs, A. G. Slater, A. I. Cooper and F. Blanc, Ultra-Fast Molecular Rotors within Porous Organic Cages, Chem. Eur. J. **23** (2017) 1-6.

Artificial Photosynthesis: catalytic systems for the sustainable production of fuel

Alex Cowan

We develop catalysts for the sustainable production of fuels from carbon dioxide and water using renewable energy resources. This is a field sometimes called solar fuels, or artificial photosynthesis. Recent work has focused on the chemistry of carbon dioxide utilisation with programmes studying both light driven and electrochemical catalysts that can convert industrially generated waste CO_2 into useful chemical feedstocks and fuels.

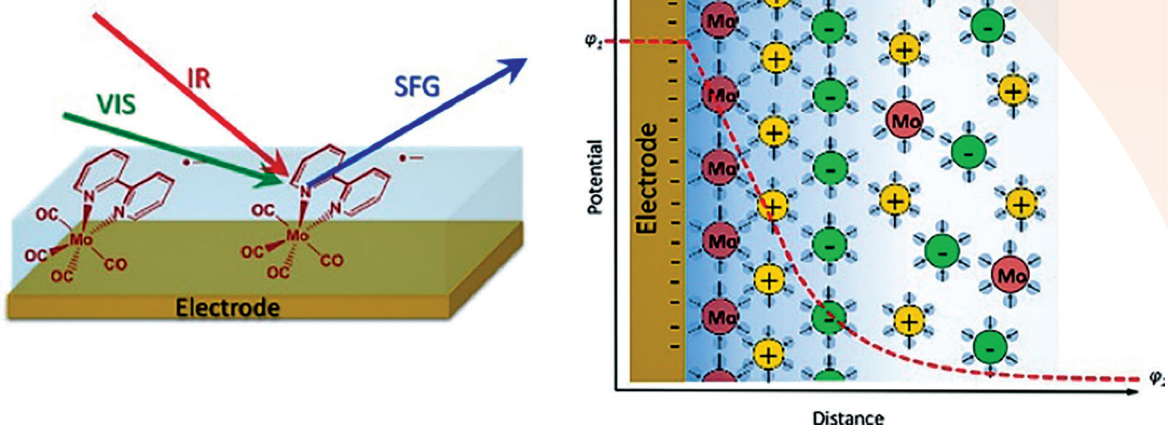
In addition to developing new catalysts for carbon dioxide utilisation and water splitting, we also have an active programme that uses laser spectroscopies to study catalytic mechanisms. In particular we have expertise in transient absorption spectroscopy, a technique that enables the study of light induced processes, and vibrational sum-frequency generation spectroscopy, a powerful tool for the study of surface mechanisms and interfacial processes.

Highlight: Understanding the factors controlling CO_2 reduction at an electrode surface

The electrochemical reduction of carbon dioxide offers a route to generating sustainable carbon fuels. Therefore intense effort is being dedicated world-wide to developing new materials and catalysts that can make the process more efficient. A problem limiting catalyst development has been a limited understanding of how intermediates interact on an electrode. Although such surface species can be short-lived and hard to detect under operating conditions they are believed to be critical in controlling activity.

Working in collaboration with the UK Central Laser Facility we have reported how vibrational sum frequency generation (VSFG) spectroscopy, a technique which selectively probes molecules at interfaces, can be used to monitor CO_2 reduction catalysis at electrode surfaces in real-time.

These first studies demonstrated the vital role of electrode-catalyst interactions in enabling efficient CO_2 reduction with a particular catalyst, Mo(bpy)$(CO)_4$, and we are now expanding our work to identify the design features required for efficient catalysis.



VSFG spectroscopy is a laser based technique that selectively probes molecules at interfaces. Here we have demonstrated how it can be used to follow the mechanism of carbon dioxide reduction at an electrode surface. Published under a Creative Commons Attribution License in J. Am. Chem. Soc. ***139****, 13791-13797 (2017).*

G. Neri, P. M. Donaldson and A. J. Cowan, The role of electrode-catalyst interactions in enabling efficient CO_2 reduction with Mo(bpy)$(CO)_4$ as revealed by vibrational sum-frequency generation spectroscopy, J. Am. Chem. Soc. **139**, 13791-13797 (2017).

Photoemission Characterisation of Materials for Electronic Devices and Renewable Energy Applications

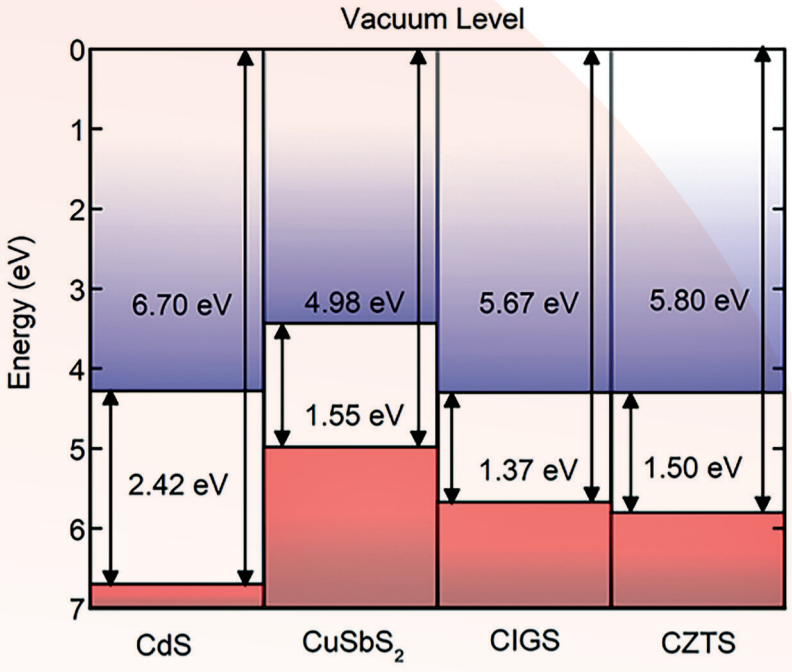
Vin Dhanak

Our interests are in solar conversion and battery storage materials as well as gate dielectrics for both low and high power metal-oxide-semiconductor field-effect transistors. Photoemission and inverse photoemission are used to measure the chemical and electronic properties of a range of materials with applications in electronic devices and energy materials. The measurements elucidate not only composition and oxidation states, but also band line-up determination at interfaces and its relation to other physical properties. We also synthesise CZTS and related PV absorber materials by chemical bath deposition, spray pyrolysis and magnetron sputtering. In addition, the ultrahigh vacuum systems in our laboratory also have scanning tunnelling microscopy and low energy electron diffraction capabilities for surface studies.

Highlight: Electronic Structure of $CuSbS_2$ for Use as a Photovoltaic Absorber

Copper antimony sulphide (CAS) demonstrates favourable solar matched band gap and high absorption coefficient, and is considered a good potential solar cell absorber. However, to date, this earth abundant material has seen relatively poor solar cell performance when used in the common cell architecture using CdS buffer layers as used in $CuInGaSe_2$ (CIGS) solar cells. We used phase pure CAS and showed that a careful analysis of the core-level spectra reveals how XPS can play a valuable role in characterising the material, and determining the effects of contaminants. A comparison of the valence band spectra with DFT calculations of the density of states shows how states arising from the Sb cation lie underneath states from the Cu cation. The effect raises the valence band maximum, with the consequence that the conduction band is misaligned with CdS, and is the reason for the poor performance of cells using a CAS/CdS heterojunction. The study shows that using a greater knowledge of the underlying electronic structure in materials like CAS can help in a redesign of solar cell architecture.

T. J. Whittles, T. D. Veal, C. N. Savory, A. W. Welch, F. Willian de Souza Lucas, J. T. Gibbon, M. Birkett, R. J. Potter, D. O. Scanlon, A. Zakutayev, and V. R. Dhanak, Core Levels, Band Alignments, and Valence-Band States in $CuSbS_2$ for Solar Cell Applications, ACS Applied Materials & Interfaces **9**, 41916 (2017).



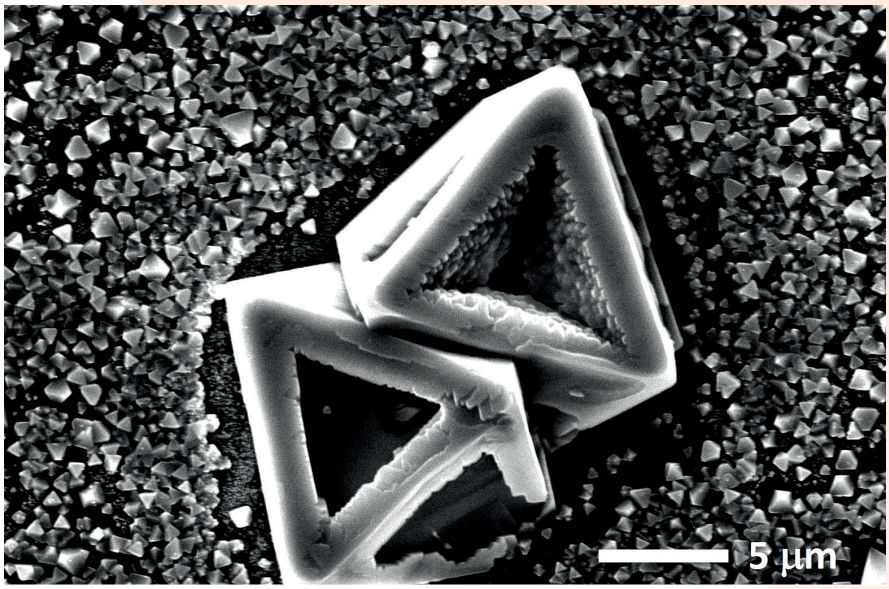
Vacuum level-aligned band diagram for $CuSbS_2$ from ionisation potential measurements using XPS and band gap from optical absorption. The band line-up is compared with other common absorbers and the common n-type window layer material, CdS. Literature values of ionisation potential and band gap are taken for CdS, CIGS and CZTS. The figure illustrates the misalignment of $CuSbS_2$ band extrema and the reason for the poor performance of cells using CIGS architecture where CdS is used as the buffer layer. Reproduced from T. J. Whittles, PhD thesis, 2017.

Solar energy materials and solar cells
Ken Durose

This group develops new and emerging materials for solar photovoltaics and also demonstrates and develops working solar cells from them. We have facilities for making a wide range of thin films of inorganic and organic materials including by sputtering, close space sublimation, evaporation and spin coating. This allows us to create research samples of both new and emerging materials allowing their optical, electrical and structural properties to be investigated. Our dedicated laboratory is then capable of making full solar PV devices from them to evaluate both their solar conversion efficiency and the underlying physical effects that may be exploited to maximise their efficiency. Presently we are working on transparent conductors, inorganic thin film absorbers including CdTe, Sb_2Se_3, all-inorganic perovskites including $CsPbI_2Br$ and Cs_2TeI_6 and organic partner layers for use in heterostructures or as electrical contacts.

Highlight: An all-inorganic perovskite for solar cell applications

Postdoc Isabel Vazquez Fernandez worked on a novel perovskite structured material to evaluate its potential for use in practical solar cell devices. The last few years have seen the 'perovskites revolution' – the emergence of a new class of hybrid organic-inorganic materials that have achieved high efficiencies more rapidly than any other material in the history of solar photovoltaics. However, despite their successes, these materials suffer from instability in light and with water vapour. Efforts to commercialise them will have to overcome significant technical obstacles. The alternative approach of Dr Vazquez Fernandez is to use a wholly inorganic material which should be more stable: Cs_2TeI_6 was identified from theoretical studies as a possible candidate and there are very few experimental studies on it to date. The first challenge was to make thin film samples – her first attempts using spin coating created some beautiful trigonal bi-pyramidal structures (see image), but these were not appropriate for making PV devices. Recent refinements to the recipe have generated the required flat films, and these are undergoing extensive electrical and optical evaluation in preparation for making working devices.



Self-assembled trigonal bi-pyramidal crystals of Cs_2TeI_6 formed by spin coating. Isabel Vazquez Fernandez, unpublished.

Atomic structure/charge distribution at the electrochemical interface
Yvonne Gründer

Electrochemical interfaces play a crucial role in many systems used for clean energy production, conversion and storage as well as for material processing. The structure of the electrode and electrolyte, as well as stability effects and charge transfer mechanism are the underlying properties and processes which can crucially affect reactivity and performance of electrochemical applications.

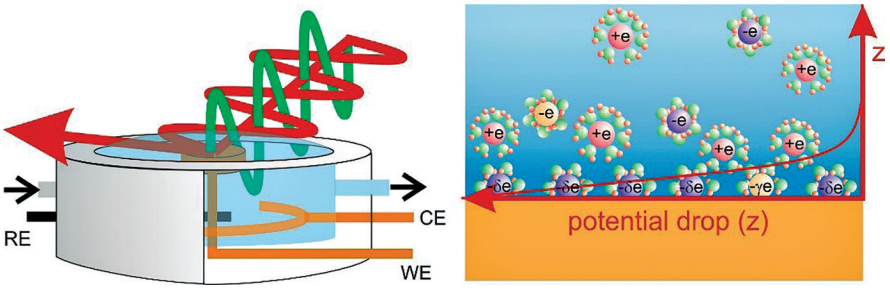
We employ in-situ surface X-ray diffraction to enable an atomic/molecular-level understanding of the interface under reactive conditions. A combination of X-ray diffraction and spectroscopy and the development of new experimental set-ups allow us to characterise electrochemical interfaces in-situ, including its potential and time dependence, in order to link structure, reactivity and stability.

Highlight: Charge Distribution at the electrochemical Interface

In-situ studies of the chemical bonding are rather difficult due to the presence of the electrolyte, as standard characterisation techniques which are mostly ultra-high vacuum-based cannot be applied. We have successfully employed resonance surface diffraction, a combination of X-ray spectroscopy and X-ray diffraction to gain site specific information about the charge distribution at a buried interface. The development of a theoretical tool further elucidated the charge transfer and bond formation at a polarised solid-liquid interface.

The adsorption of halide anions onto Cu and Au single crystal electrode surfaces reveals that there is significant modification of the charge distribution induced by a $3d_{z^2}$-$4p_z$ hybridisation of the electrons of the subsurface copper atom.

The ab initio simulation enables a direct comparison of the charge distribution models to the experimental results. This has potential impact both in further developing the theoretical understanding of the interface structure and in designing new materials for electrochemical applications.



The electrochemical cell and the two polarisations of the incident X-ray beam, normal to the surface (green line) and in the surface plane (red line). Model of the electrochemical interface with the ions in solution and adsorbed on the surface and the current understanding of partial charges together with the potential drop across the interface. Reproduced with permission. Copyright Royal Society of Chemistry, 2017.

Y. Joly, A. Abisset, A. Bailly, M. De Santis, F. Fettar, S. Grenier, Y. Gründer, Simulation of Surface Resonant X-ray Diffraction. Journal of Chemical Theory and Computation **14**, 973-980 (2018). Y. Gründer, and C. A. Lucas, Probing the charge distribution at the electrochemical interface, Phys. Chem. Chem. Phys. **19**, 8416-8422 (2017).

Advanced In situ Characterisation of Battery Materials

Laurence Hardwick

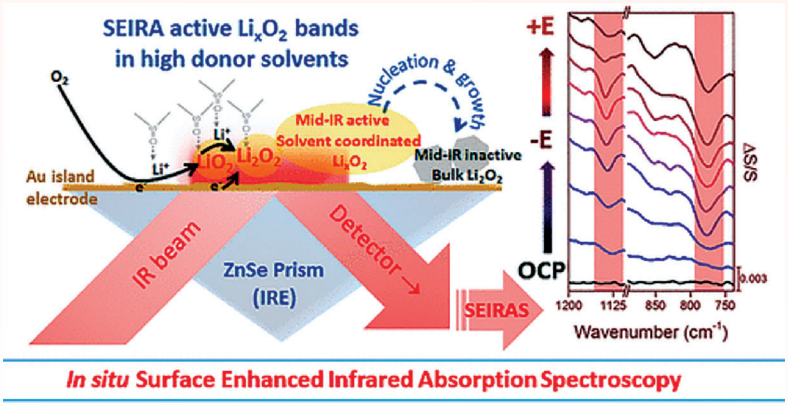
Lithium ion batteries have revolutionised technological progress of the past two decades; however, there appears to be little room left to increase further their specific energy. Developing new types of batteries with higher energy storage and superior performance is crucial for the realization of a true alternative to a fossil-fuel-based energy economy. In view of the overwhelmingly high gravimetric energy densities projected by theoretical as well as recent experimental reports, metal-oxygen ($M\text{-}O_2$) batteries based on lithium, sodium, potassium or calcium; popularly known as metal-air batteries, promise to lead next-generation energy storage systems.

Our group's research focusses on fundamental studies providing molecular level understanding and mechanistic insight into the underlying interfacial electrode processes during discharge-charge (electro)chemistry, as well as other desirable or undesirable reaction pathways, are required in order for $M\text{-}O_2$ batteries to develop into a technology of the near future. We do this through a combination of *in situ* and *ex situ* electrochemical, Raman, infrared and UV-visible spectroscopy, and X-ray photoelectron spectroscopies.

Highlight: In Situ Surface-Enhanced Infrared Spectroscopy to Identify Oxygen Reduction Products in Nonaqueous Metal-Oxygen Batteries

The complexity and sensitivity of the discharge/charge reactions recognized by recent reports underline the importance of detailed, theoretical as well as experimental, mechanistic investigations under controlled conditions in order to fill in the knowledge gap hampering $M\text{-}O_2$ battery technology.

In the context of developing high energy storage metal-oxygen ($M\text{-}O_2$) batteries, the precise reaction mechanisms of oxygen with metal ions in non-solvents remains poorly understood. We report on the detection of metastable, solvated, and surface adsorbed alkali ($M\text{-}O_2$) discharge species using in situ attenuated total reflectance surface enhanced infrared absorption spectroscopy (ATR-SEIRAS). Oxygen-oxygen stretching bands, ν(O-O), of superoxide species formed during $M\text{-}O_2$ battery discharge have been challenging to observe by conventional infrared (IR) techniques, and because of this, there has been limited use of IR techniques for in situ monitoring of the discharge products at the cathode in metal-O_2 batteries. Our work established that certain stretching bands, ν(M-O) and ν(O-O), of metal (lithium and sodium) superoxide and peroxide molecular species are IR active, although these vibrational modes are silent or suppressed in their crystalline forms. An in situ IR spectroscopy based approach to distinguish between "solution mediated" and "surface confined" discharge pathways in non-aqueous $M\text{-}O_2$ batteries is demonstrated.



*Using in situ infrared spectroscopy we are able to detect metastable, solvated, and surface adsorbed metal peroxide and superoxide species. Published under a Creative Commons Attribution License in J. Phys. Chem C **121**, 19657-19667 (2017).*

Padmanabhan Vivek, N. G. Berry, J. Zou, R. J. Nichols, L. J. Hardwick, In Situ Surface-Enhanced Infrared Spectroscopy to Identify Oxygen Reduction Products in Nonaqueous Metal-Oxygen Batteries, J. Phys. Chem. C, **121** 19657-19667 (2017).

Hybrid nanomaterials for renewable energy, nanoplasmonics and nanophotonics

Frank Jäckel

Hybrid nanomaterials combine different material classes (i.e. metals, semiconductors, organics) on the nanoscale. Nanomaterials themselves can already display properties significantly different from their bulk counterparts due to quantum confinement effects. Hybrid nanomaterials on the other hand can exhibit novel or enhanced properties that neither of the components exhibits itself.

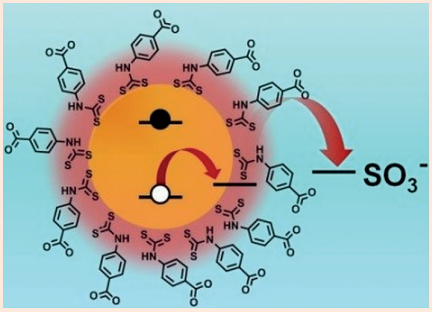
We are interested in the preparation and fundamental photophysical characterisation of hybrid nanomaterials for applications in renewable energy, nanoplasmonics and nanophotonics.

Hybrid metal-semiconductor nanomaterials can be used for photocatalytic hydrogen generation and other solar fuels as part of a green and sustainable energy supply. We are interested in developing novel hybrid nanomaterials for photocatalysis and in understanding their fundamental photophysics.

Hybrid metal-organic nanomaterials can be used to manipulate a range of material properties and processes by making use of their localised surface plasmon resonances. We are particularly interested in manipulating processes such as Raman scattering, and charge and energy transfer.

Highlight: Hydrophilic, Hole-Delocalizing Ligand Shell to Promote Charge Transfer from Colloidal CdSe Quantum Dots in Water

Colloidal semiconductor nanocrystals are attracting interest for applications in photocatalytic applications as scalable and cheap materials with tuneable optical and electronic properties. One challenge for their application however is the presence of stabilising ligand shells. While these shells provide stability, they also present a steric barrier that hinders surface access for photocatalytic reactions. In this work, we investigate a more dynamic ligand shell that provides both stability to the nanocrystals and the promotion of charge transfer required for photocatalytic reactions. We use transient absorption spectroscopy to study CdSe quantum dots functionalized with hydrophilic, hole-delocalizing dithiocarbamate ligands in water and find that conjugated ligands facilitate charge transfer to redox species in solution.



Cartoon representation of a semiconductor nanocrystal stabilised by a redox active ligand shell that provides a charge transfer pathway for photogenerated holes to redox active species in solution. Reproduced with permission. Copyright American Chemical Society 2017.

J. R. Lee, W. Li, A. J. Cowan, F. Jäckel, A Hydrophilic, Hole-Delocalizing Ligand Shell to Promote Charge Transfer from Colloidal CdSe Quantum Dots in Water, J. Phys. Chem. C **121**, 15160-15168 (2017).

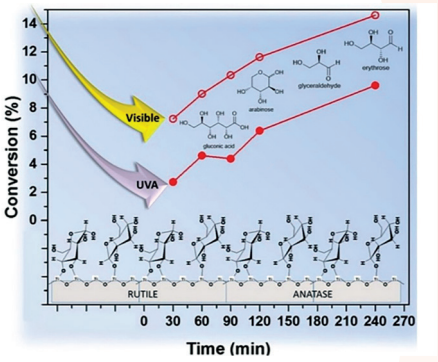
Catalysis for Sustainable Chemistry

Tony Lopez-Sanchez

We utilise our expertise in Catalysis to address Green Chemistry and Energy reactions. We are particularly interested in developing new catalysts and efficient routes to renewable chemicals from biomass and CO_2. We believe that some of these targets will require the development of new advanced materials and we are developing these materials in partnership with colleagues in other disciplines. In particular we are studying novel nanostructured oxides, semiconductors, metal nanoparticles and porous polymers using high-throughput (HT) automated instruments for synthesis, characterisation and testing. We are also exploring the application of non-conventional technologies such as photocatalysis and microwaves for some of these applications. In addition to rapid discovery, we believe that high-throughput discovery if coupled with spectroscopy and HT characterisation, can generate more fundamental advances, such as developing structure-activity relationships in catalysis.

Highlight: Visible light selective photocatalytic conversion of glucose by TiO_2

We report the visible-light mediated selective photo-oxidation of glucose using unmodified TiO_2 as a catalyst. The effect of the catalyst to substrate ratio, lamp power and TiO_2 crystalline phases on the conversion and product distribution under both visible and UVA light is explored. Higher conversions were obtained under UVA light but as a result of substantial mineralization through an unselective pathway. Optimization of the reaction conditions resulted in 42% glucose conversion under visible light with 7% selectivity to gluconic acid and 93% selectivity to other partial oxidation products with the total suppression of a mineralization pathway to CO_2. It is also shown that selective glucose conversion can occur under natural sunlight light after 7 h exposure. In this systematic study, we prove that it is indeed possible to use TiO_2 as a photocatalyst to upgrade biomass derivatives selectively by tailoring the reaction conditions. Most importantly, we find the ligand-to-metal charge-transfer effect as a result of glucose adsorption to the surface of TiO_2 determinant in the photo-activity observed under visible light irradiation. Knowledge of this effect along with the careful control of reaction conditions means that the selective photo-catalytic conversion of other biomass derived carbohydrates under visible light is a viable route to higher value chemicals.



*Published under a Creative Commons Attribution License in Applied Catalysis B: Environmental **202** (2017) 281.*

Thin film solar cell devices and materials

Jon Major

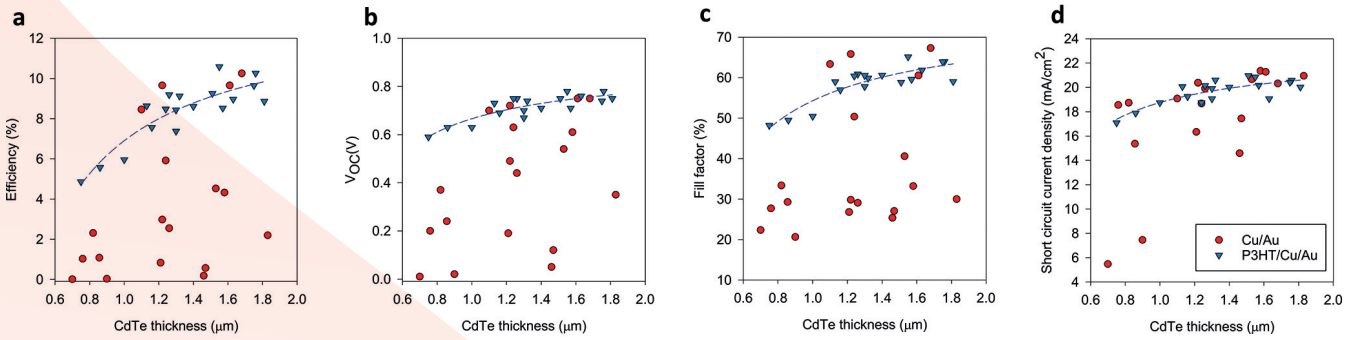
Thin film solar cells are now established as an industrial technology, but there remains tremendous scope for improving performance and reducing cost. Our research focusses on developing new solar cell structures and process to develop the technology. We combine device level characterisation of power output and spectral performance with materials and defect analysis to identify key limitations. Currently, we are working on new process approaches for CdTe solar cells and the development of emerging Sb_2Se_3 solar cells.

Highlight: P3HT as a Pinhole Blocking Back Contact for CdTe Thin Film Solar Cells.

This work demonstrates the use of an organic semiconductor, deposited by a solution process, as a way to block pinholes and improve performance in thin film CdTe solar cells. By adding the compound P3HT this drastically improved the fraction of working solar cells.

J. D. Major, L. J. Phillips, M. Al Turkestani, L. Bowen, T. J. Whittles, V. R. Dhanak and K. Durose. P3HT as a Pinhole Blocking Back Contact for CdTe Thin Film Solar Cells, Solar Energy Materials and Solar Cells **172**, 1-10 (2017).

*a) to d) show improvement in uniformity of cell performance parameters as a function of CdTe thickness for cells with a standard Cu/Au contact and with the addition of pinhole blocking P3HT. Published under a Creative Commons Attribution License in Solar energy materials and Solar Cells **172**, 1-10 (2017)*



Organometallic chemistry and homogeneous catalysis for sustainable organic synthesis

Alexey G. Sergeev

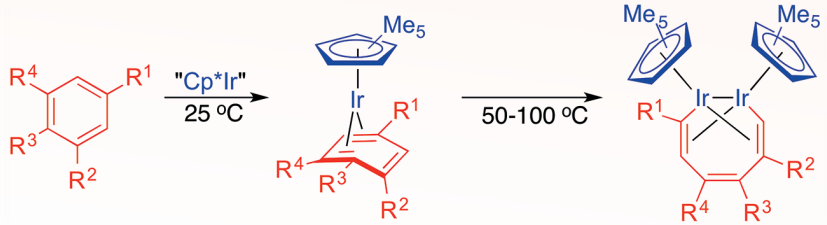
Catalysis plays a critical role for mild, clean and safe synthesis of complex chemicals from natural resources. In this context, particularly important is the functionalization of C-H and C-C bonds, the most common bonds found in both renewable and non-renewable natural resources. These bonds, however, are notoriously difficult to engage in selective chemical reactions and to address this issue we design new catalysts and synthetic strategies. We focus on investigating the structure and reactivity of well-defined soluble metal complexes that show the highest activity and selectivity in activation of C-H and C-C bonds. For this purpose we use a range of experimental methods (NMR, GC, GC-MS, HR-MS and XRD) supported by density functional theory calculations.

Highlight: Activation of aromatic C-C bonds through direct insertion of iridium metal into the aromatic ring of alkyl arenes

We have discovered a new approach for mild and selective activation of aromatic hydrocarbons by metal complexes. This approach addresses a long-standing problem of cleavage of extraordinarily strong aromatic C-C bonds by a metal centre, a key step for clean and mild conversion of coal into fuel and valuable chemicals.

Specifically, we have demonstrated that the aromatic C-C bonds can be cleaved by insertion of a simple, well-defined iridium Cp*Ir fragment into the aromatic ring of industrially important alkyl arenes (see figure). This insertion occurs at unprecedently mild conditions and without observable activation of weaker C-H bonds. The know-how of this approach is the metal-induced ring strain that boosts the reactivity of the strong ring C-C bonds towards metal insertion.

Our next challenge will be to render this remarkable process catalytic and demonstrate its utility for industrially important transformations.



*Selective scission of strong arene C-C bonds by well defined metal complexes. Published under a Creative Commons Attribution License in Angew. Chem. Int. Ed. **56** 3266-3269 (2017).*

M. Jakoobi, N. Halcovitch, G. F. S. Whitehead, and Alexey G. Sergeev, Selective Arene Cleavage through Direct Insertion of Iridium into the Aromatic Ring, Angew. Chem. Int. Ed. **56,** 3266-3269 (2017).

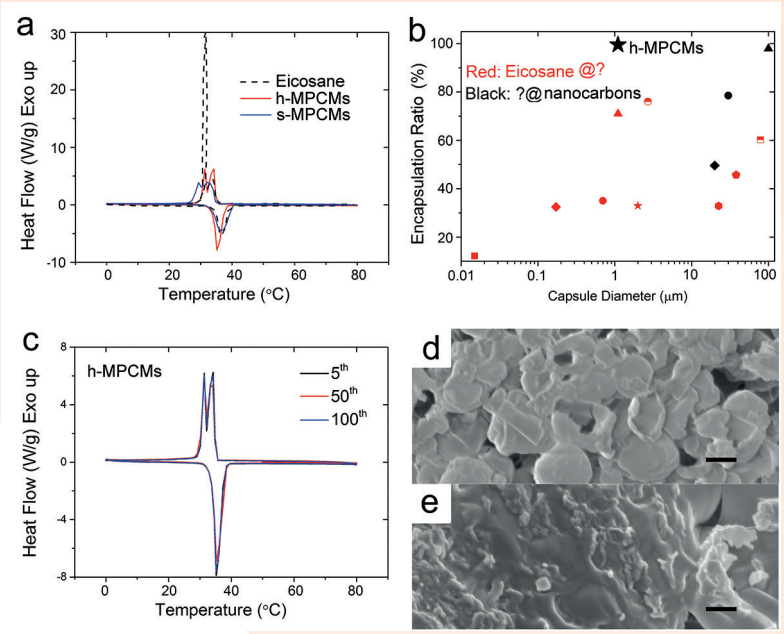
Encapsulation of active materials for energy applications

Dmitry Shchukin

Research activities include the study of the non-equilibrated interfaces, development of composite hollow nanocontainers with controlled shell permeability for encapsulation of the energy-enriched materials, drugs, biocides and corrosion inhibitors; development of nanocontainer-based feedback active surfaces for further application in active self-healing and antifouling materials, catalysis and medicine; synthesis of nanomaterials with new properties in the ultrasonic cavitation zone, synthesis of amorphous nanocomposites with enhanced (photo) catalytic performance in non-equilibrated conditions at the cavitation interface, use of the ultrasonic cavitation as new media for high-temperature chemical synthesis.

Highlight: Encapsulation of phase change materials for thermal energy storage

The performance of solar-thermal conversion systems can be improved by incorporation of nanocarbon-stabilized encapsulated phase change materials (PCMs). The geometry of PCMs in the microcapsules plays an important role for improving their heating efficiency and reliability. Yet few efforts have been made to critically examine the formation mechanism of different geometries and their effect on PCMs-shell interaction. Through changing the cooling rate of original emulsions, we acquire PCMs within the nanocarbon microcapsules with a hollow structure of PCMs (h-PCMs) or solid PCM core particles (s-PCMs). X-ray photoelectron spectroscopy and atomic force microscopy reveals that the capsule shell of the h-PCMs are enriched with nanocarbons and have a greater PCMs-shell interaction compared to s-PCMs. This results in the h-PCMs being more stable and having greater heat diffusivity within and above the phase transition range than the s-PCMs do. The geometry-dependent heating efficiency and system stability may have important and general implications for the fundamental understanding of heat generating systems.



Heating performance of h- and s-PCMs. (a) DSC curves of the eicosane, h-PCMs and s-PCMs at the second endothermic and exothermic cycle. (b) Plot of encapsulation efficiency against capsule shell thickness for the shape-stable MPCMs in (a) and from literature results (red and black dots). Red: Eicosane@? means eicosane core is stabilised by non-nanocarbon shell materials, and black: ?@nanocarbons is for the nanocarbon-stabilised PCM other than eicosane. (c) A collection of DSC curves of the h-MPCMs tested at 5th, 50th and 100th cycles, showing the stable encapsulation during endothermic and exothermic processes. (d) and (e) are SEM images of h- and s-MPCMs after the endothermic and exothermic cycles. Scale bar: 1 μm. Published under a Creative Commons Attribution License in Z. Zheng et al. ACS Nano, 11 (2017) 721.

Z. Zheng, Z. Chang, G.-K. Xu, F. McBride, A. Ho, Z. Zhuola, M. Michailidis, W. Li, R. Raval, R. Akhtar, D. G. Shchukin. Microencapsulated Phase Change Materials in Solar-Thermal Conversion Systems: Understanding Geometry-Dependent Heating Efficiency and System Reliability, ACS Nano **11** 721-729 (2017).

Chemically Selective Alternatives to Photoferroelectrics for Polarization-Enhanced Photocatalysis: the Untapped Potential of Hybrid Inorganic Nanotubes

Gilberto Teobaldi

Photocatalytic materials (photocatalysts, PCs) can exploit solar light energy for chemical fuels production, pollutant degradation, or to access alternative, highly selective, reaction paths to high-value chemicals. The basic requirements of good (visible) light-absorbance, efficient separation of photogenerated electron-hole (e-h) pairs, independent e (h) diffusion to the PC-surfaces and transfer to (different or selected) reactants, are clearly established.

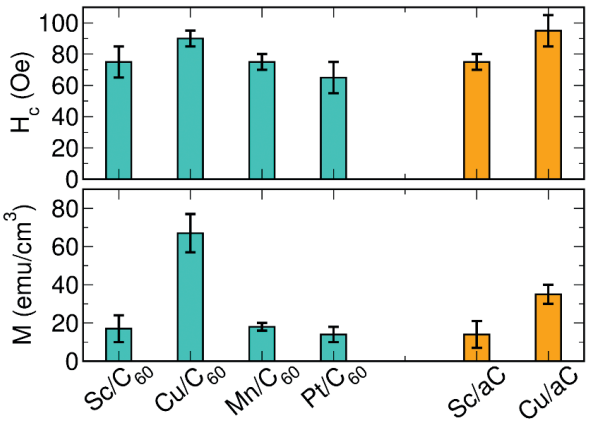
However, fulfilment of such requirements by cheap and scalable materials remains elusive due to the poorly understood relationships between the properties of a PC and its atomic composition, structure, and solvent-dependent interactions with reactants.

Aiming at efficient e-h separation and diffusion to reactants, both one-dimensional (1D) structuring of PCs and use of permanently polarised photoferroelectrics have started to be explored and found to increase photocatalytic performance. Confinement of reactants inside nano-porous PCs has also been observed to benefit reaction selectivity. These, to date disconnected, advances raise the question as to whether the benefits of these different strategies could be integrated into one, ideally cheap, material.

Atomistic simulations of existing hybrid organic-inorganic nanotubes (NTs) suggest

this to be the case. Based on the theoretical insights, generalisable strategies are proposed to increase the NT-polarisation for maximally enhanced electron-hole separation, while modulating independently the electrostatics inside the NT cavity, thence the electronic alignment with reactants and the e(h)-transfer kinetics.

Separate control of cavity electrostatics and polarisation-enhanced electron-hole separation may enable innovative strategies based on the use of local-polarisations in overall dipole-free (chemically selective) NTs to force reactants to match the photo-catalyst, as opposed to standard band-engineering of photo-catalysts for a given reactant.



Permanent dipole density ($\mu\sigma$) at the wall of open-ended, water-soluble inorganic imogolite nanotubes, and related interface potential step (ΔV), resulting in an electronegative cavity and an electropositive outer surface. These can be used to perturb interacting species (reactants, products and catalysts), their electronic levels and wavefunctions, therefore the overall energy drive and kinetics of the redox event. Published under a Creative Commons Attribution License in J. D. Elliott et al., Adv. Sci. 3, 1600153 (2016).

J. D. Elliott, E. Poli, I. Scivetti, L. E. Ratcliff, L. Andrinopoulos, J. Dziedzic, N. D. M. Hine, A. A. Mostofi, C. K. Skylaris, P. D. Haynes and G. Teobaldi, *Chemically Selective Alternatives to Photoferroelectrics for Polarization-Enhanced Photocatalysis: The Untapped Potential of Hybrid Inorganic Nanotubes*. Adv. Sci. **3**, 1600153 (2016).

Semiconductor material physics for renewable energy applications

Tim Veal

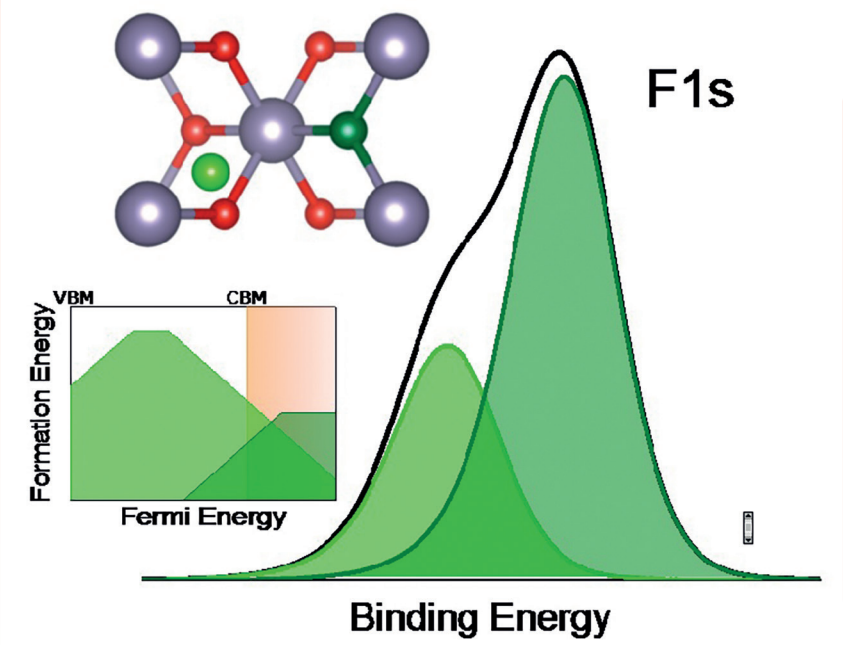
Novel semiconductor materials are important for a low carbon future, including the sustainable terawatt scale-up of thin film solar cells and for energy efficiency technologies. Our experimental approach of combining optical, electronic, defect and photoemission characterisation of semiconductors enables the development of new advanced materials and understanding for future sustainable energy technologies. Particular current focusses include novel dopants in transparent conducting oxides, ultra-thin metal layers as transparent conductors, new photovoltaic absorber materials and band alignment measurement and design in solar cells.

Highlight: Discovery points the way to better and cheaper transparent conductors

In a collaboration with NSG Group's (Pilkington's) European Technology Centre and University College London, we have made a discovery that could improve the conductivity of a type of glass coating which is used on items such as touch screens, energy efficient windows and thin film solar cells.

Coatings are applied to the glass of these items to make them electrically conductive whilst also allowing light through. Fluorine doped tin dioxide is one of the materials used in commercial low cost glass coatings but it turns out that tin dioxide has as yet untapped potential for improved performance.

We identified that interstitial fluorine atoms limit the conductivity of fluorine doped tin dioxide, as they partially compensate substitutional fluorine donors and increase free carrier scattering. The next step is to address the challenge of finding alternative novel dopants that avoid these inherent drawbacks.



*Photoemission spectroscopy of the F 1s core level was used to identify the presence of substitutional and interstitial fluorine in a 2:1 ratio which was correlated with transport, optical and theoretical results. Published under a Creative Commons Attribution License in Adv. Funct. Mater. **28** (2018) 1701900.*

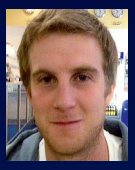
J. E. N. Swallow, B. A. D. Williamson, T. J. Whittles, M. Birkett, T. Featherstone, N. Peng, A. Abbott, M. Farnworth, K. J. Cheetham, P. Warren, D. O. Scanlon, V. R. Dhanak, and T. D. Veal Self-Compensation in Transparent Conducting F-doped SnO_2 Adv. Funct. Mater. **28** (2018) 1701900

PhD Theses in 2017

Dr Arturas Adomkevicius

Controlling Transition Metal Oxides Nanostructures for Energy Storage Systems

Supervisor: Laurence Hardwick and Chi-Chang Hu (NTHU)



Dr Tom Galloway

Shining Light on Electrode Interfaces

Supervisors: Laurence Hardwick and Sarah Ball (Johnson Matthey)

Dr Lorena Martin Olivera

Density Functional Theory screening of molecular strategies for emergent magnetism at Copper interfaces

Supervisors: Dmitry Shchukin and Gilberto Teobaldi

Dr Elizabeth Cocklin

Surface X-ray Diffraction Studies of Electrode/ Vacuum and Electrode/ Electrolyte Interfaces

Supervisors: David Martin and Chris Lucas

Dr Michael Graham

Encapsulated Salt Hydrate Phase Change Materials for Thermal Energy Storage

Supervisor: Dmitry Shchukin

Dr Giorgios Papageorgiou

Nano- and Micro-structured CdTe Solar Cells

Supervisor: Ken Durose

Dr Ebenezer Tetsi

AB_2O_6 oxides: potential thermoelectric and magnetic materials

Supervisor: Jon Alaria

Dr Nor Azam Bin Endot

Selective hydrogenation of 5-hydroxymethylfurfural (HMF) to 2, 5-dimethylfuran (DMF) over Ru, Ni, and Co mono and bimetallic catalysts supported on carbon and carbon nanotubes

Supervisor: Tony Lopez-Sanchez

Dr Jon Lee

Tailoring the ligand shell of quantum dots towards improved photocatalytic charge transfer

Supervisors: Frank Jäckel and Alex Cowan

Dr Annette Pressman

Electrical properties of cadmium telluride thin film solar cells activated with magnesium chloride

Supervisor: Ken Durose

Dr Marta Fernández Giménez

Iridium-catalysed cleavage and formation of unstrained aliphatic carbon-carbon bonds

Supervisor: Alexey Sergeev

Dr Gaia Neri

The photo- and electrochemical reduction of carbon dioxide mediated by molecular catalysts

Supervisor: Alex Cowan

Dr Aldo Reyes

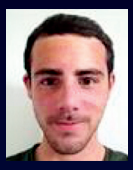
Synthesis, Promotion and Characterization of Imogolite Materials as Heterogeneous Catalysts and Photocatalysts

Supervisor: Tony Lopez-Sanchez

Dr Thomas Whittles

Electronic Characterisation of Earth-Abundant Sulphides for Solar Photovoltaics

Supervisor: Vin Dhanak



Dr Mark Forster

Time-resolved spectroscopic studies of hematite photoelectrodes for photoelectrochemical water splitting

Supervisor: Alex Cowan

Dr Nadiah Mohamad Noh

Catalytic Route for the Synthesis of Cyclic Organic Carbonates from Renewable Polyols

Supervisor: Tony Lopez-Sanchez

Dr Chris Sole

Electrochemical Energy Storage with Graphene-Enabled Materials

Supervisor: Laurence Hardwick

Publications by SIRE academic staff in 2017

Jonathan Alaria

L. M. Daniels, S. N. Savvin, M. J. Pitcher, M. S. Dyer, J. B. Claridge, S. Ling, B. Slater, F. Corà, J. Alaria, and M. J. Rosseinsky
Phonon-glass electron-crystal behaviour by A site disorder in n-type thermoelectric oxides.
Energy Environ. Sci. **10**, 1917-1922 (2017)

Q. D. Gibson, M. S. Dyer, G. F. S. Whitehead, J. Alaria, M. J. Pitcher, H. J. Edwards, J. B. Claridge, M. Zanella, K. Dawson, T. D. Manning, V. R. Dhanak, and M. J. Rosseinsky
$Bi_4O_4Cu_{1.7}Se_{2.7}Cl_{0.3}$: Intergrowth of BiOCuSe and Bi_2O_2Se Stabilized by the Addition of a Third Anion
J. Am. Chem. Soc. **139**, 15568-15571 (2017)

H. C. Sansom, G. F. S. Whitehead, M. S. Dyer, M. Zanella, T. D. Manning, M. J. Pitcher, T. J. Whittles, V. R. Dhanak, J. Alaria, J. B. Claridge, and M. J. Rosseinsky
$AgBiI_4$ as a Lead-Free Solar Absorber with Potential Application in Photovoltaics
Chem. Mater. **29**, 1538-1549 (2017)

J. F. Shin, H. Niu, J. Alaria, J. B. Claridge, and M. J. Rosseinsky
Substitution of Re^{7+} into $CaMnO_3$: an efficient free electron generation dopant for tuning of thermoelectric properties Physical Chemistry Chemical Physics **19**, 30781-30789 (2017)

Frédéric Blanc

F. Blanc
Acidity Strength of Solid Catalysts Probed by Hyperpolarized Natural Abundance ^{17}O NMR Spectroscopy
Angew. Chem. Int. Ed. **56**, 11694-11696 (2017); Angew. Chem. **129**, 11854-11856 (2017)

F. Blanc
Investigation of Catalytic Surfaces with Surface-Enhanced Solid-State NMR Spectroscopy
In B. Sels and M. Van de Voorde (Eds), Nanotechnology in Catalysis: Applications in the Chemical Industry, Energy Research, and Environment Protection, pp. 1003-1028 (Wiley, 2017)

N. J. Brownbill, D. Gajan, A. Lesage, L. Emsley, and F. Blanc
Oxygen-17 dynamic nuclear polarisation enhanced solid-state NMR spectroscopy at 18.8 T
Chem. Comm. **53**, 2563-2566 (2017)

I. R. Colinas, K. K. Inglis, F. Blanc, and S. R. J. Oliver
Anion exchange dynamics in the capture of perchlorate by a cationic Ag-based MOF.
Dalton Transactions **46**, 5320-5325 (2017)

R. Giovine, C. Volkringer, M.-A. Springuel-Huet, A. Nossov, F. Blanc, J. Trebosc, T. Loiseau, J.-P. Amoureux, O. Lafon, and F. Pourpoint
Study of Xenon Mobility in the Two Forms of MIL-53(Al) Using Solid-State NMR Spectroscopy
J. Phys. Chem. C **121**, 19262-19268 (2017)

A. R. Hughes, N. J. Brownbill, R. C. Lalek, M. E. Briggs, A. G. Slater, A. I. Cooper, and F. Blanc
Ultra-Fast Molecular Rotors within Porous Organic Cages
Chemistry – A European Journal **23**, 17217-17221 (2017)

G. Kim, J. M. Griffin, F. Blanc, D. M. Halat, S. M. Haile, and C. P. Grey
Revealing Local Dynamics of the Protonic Conductor $CsH(PO_3H)$ by Solid-State NMR Spectroscopy and First-Principles Calculations
J. Phys. Chem. C **121**, 27830-27838 (2017)

D. Stewart, D. Antypov, M. S. Dyer, M. J. Pitcher, A. P. Katsoulidis, P. A. Chater, F. Blanc, and M. J. Rosseinsky
Stable and ordered amide frameworks synthesised under reversible conditions which facilitate error checking
Nat. Commun. **8**, 1102 (2017)

D. Xiao, S. Xu, X. Han, X. Bao, Z. Liu, and F. Blanc
Direct structural identification of carbenium ions and investigation of host-guest interaction in the methanol to olefins reaction obtained by multinuclear NMR correlations
Chemical Science **8**, 8309-8314 (2017)

Alex Cowan

M. Forster and A. J. Cowan
Rationalizing the Efficiency of Hydrogen-Treated TiO_2 Nanomaterials in Light Driven Water-Splitting Applications
In Xiaobo Chen and Yi Cui (Eds), Black TiO_2 Nanomaterials for Energy Applications (World Scientific, 2017); pp. 215-248.

J. R. Lee, W. Li, A. J. Cowan, and F. Jäckel
Hydrophilic, Hole-Delocalizing Ligand Shell to Promote Charge Transfer from Colloidal CdSe Quantum Dots in Water
J. Phys. Chem. C **121**, 15160-15168 (2017)

G. Neri, P. M. Donaldson, and A. J. Cowan
The Role of Electrode-Catalyst Interactions in Enabling Efficient CO_2 Reduction with $Mo(bpy)(CO)_4$ as Revealed by Vibrational Sum-Frequency Generation Spectroscopy
J. Am. Chem. Soc. **139**, 13791-13797 (2017)

M. C. Nolan, J. J. Walsh, L. L. E. Mears, E. R. Draper, M. Wallace, M. Barrow, B. Dietrich, S. M. King, A. J. Cowan, and D. J. Adams
pH dependent photocatalytic hydrogen evolution by self-assembled perylene bisimides
J. Mater. Chem. A **5**, 7555-7563 (2017)

D. J. Woods, R. S. Sprick, C. L. Smith, A. J. Cowan, and A. I. Cooper
A Solution-Processable Polymer Photocatalyst for Hydrogen Evolution from Water
Adv. Energy Mater. **7**, 1700479 (2017)

X. Xiong, M. Forster, J. D. Major, Y. Xu, and A. J. Cowan
Time-Resolved Spectroscopy of ZnTe Photocathodes for Solar Fuel Production
J. Phys. Chem. C **121**, 22073-22080 (2017)

Vin Dhanak

M. Birkett, C. N. Savory, A. N. Fioretti, P. Thompson, C. A. Muryn, A. D. Weerakkody, I. Z. Mitrovic, S. Hall, R. Treharne, V. R. Dhanak, D. O. Scanlon, A. Zakutayev, and T. D. Veal
Atypically small temperature-dependence of the direct band gap in the metastable semiconductor copper nitride Cu_3N
Phys. Rev. B **95** 115201 (2017)

Q. D. Gibson, M. S. Dyer, G. F. S. Whitehead, J. Alaria, M. J. Pitcher, H. J. Edwards, J. B. Claridge, M. Zanella, K. Dawson, T. D. Manning, V. R. Dhanak, and M. J. Rosseinsky
$Bi_4O_4Cu_{1.7}Se_{2.7}Cl_{0.3}$: Intergrowth of BiOCuSe and Bi_2O_2Se Stabilized by the Addition of a Third Anion
J. Am. Chem. Soc. **139**, 15568-15571 (2017)

B. Kiss, T. D. Manning, D. Hesp, C. Didier, A. Taylor, D. M. Pickup, A. V. Chadwick, H. E. Allison, V. R. Dhanak, J. B. Claridge, J. R. Darwent, and M. J. Rosseinsky
Nano-structured rhodium doped $SrTiO_3$ – Visible light activated photocatalyst for water decontamination
Appl. Catal. B **206**, 547-555 (2017)

J. Jin, J. S. Wrench, J. T. Gibbon, D. Hesp, A. Shaw, I. Z. Mitrovic, N. Sedghi, L. J. Phillips, J. Zou, V. R. Dhanak, P. R. Chalker, and S. Hall
Schottky Diodes on ZnO Thin Films Grown by Plasma-Enhanced Atomic Layer Deposition
IEEE Trans. Electron Devices **64**, 1225-1230 (2017)

J. D. Major, L. J. Phillips, M. Al Turkestani, L. Bowen, T. J. Whittles, V. R. Dhanak, and K. Durose
P3HT as a pinhole blocking back contact for CdTe thin film solar cells
Sol. Energy Mater. Sol. Cells **172**, 1-10 (2017)

M. Puisto, K. Pussi, M. Alatalo, D. Hesp, V. R. Dhanak, C. A. Lucas, and Y. Gründer
LEED – IV and DFT study of the co-adsorption of chlorine and water on Cu(100)
Surf. Sci. **657**, 51-57 (2017)

H. C. Sansom, G. F. S. Whitehead, M. S. Dyer, M. Zanella, T. D. Manning, M. J. Pitcher, T. J. Whittles, V. R. Dhanak, J. Alaria, J. B. Claridge, and M. J. Rosseinsky
$AgBiI_4$ as a Lead-Free Solar Absorber with Potential Application in Photovoltaics.
Chem. Mater. **29**, 1538-1549 (2017)

K. Sawangsri, P. Das, S. N. Supardan, I. Z. Mitrovic, S. Hall, R. Mahapatra, A. K. Chakraborty, R. Treharne, J. Gibbon, V. R. Dhanak, K. Durose, and P. R. Chalker
Experimental band alignment of Ta_2O_5/GaN for MIS-HEMT applications
Microelectronic Engineering **178**, 178-181 (2017)

N. Sedghi, H. Li, I. F. Brunell, K. Dawson, R. J. Potter, Y. Guo, J. T. Gibbon, V. R. Dhanak, W. D. Zhang, J. F. Zhang, J. Robertson, S. Hall, and P. R. Chalker
The role of nitrogen doping in ALD Ta_2O_5 and its influence on multilevel cell switching in RRAM
Appl. Phys. Lett. **110**, 102902 (2017)

N. Sedghi, H. Li, I. F. Brunell, K. Dawson, Y. Guo, R. J. Potter, J. T. Gibbon, V. R. Dhanak, W. D. Zhang, J. F. Zhang, S. Hall, J. Robertson, and P. R. Chalker
Enhanced switching stability in Ta_2O_5 resistive RAM by fluorine doping
Appl. Phys. Lett. **111**, 092904 (2017)

S. Smalley, M. Lahti, K. Pussi, V. R. Dhanak, and J. A. Smerdon
Dibromobianthryl ordering and polymerization on Ag(100)
J. Chem. Phys. **146**, 184701 (2017)

T. J. Whittles, T. D. Veal, C. N. Savory, A. W. Welch, F. W. de Souza Lucas, J. T. Gibbon, M. Birkett, R. J. Potter, D. O. Scanlon, A. Zakutayev, and V. R. Dhanak
Core-Levels, Band Alignments, and Valence Band States in $CuSbS_2$ for Solar Cell Applications
ACS Applied Materials and Interfaces **9**, 41916-41926 (2017)

Ken Durose

J. D. Major, L. J. Phillips, M. Al Turkestani, L. Bowen, T. J. Whittles, V. R. Dhanak, and K. Durose
P3HT as a pinhole blocking back contact for CdTe thin film solar cells
Sol. Energy Mater. Sol. Cells **172**, 1-10 (2017)

J. D. Major, R. Tena-Zaera, E. Azaceta, L. Bowen, and K. Durose
Development of ZnO nanowire based CdTe thin film solar cells
Sol. Energy Mater. Sol. Cells **160**, 107-115 (2017)

K. Sawangsri, P. Das, S. N. Supardan, I. Z. Mitrovic, S. Hall, R. Mahapatra, A. K. Chakraborty, R. Treharne, J. Gibbon, V. R. Dhanak, K. Durose, and P. R. Chalker
Experimental band alignment of Ta_2O_5/GaN for MIS-HEMT applications
Microelectronic Engineering **178**, 178-181 (2017)

Q. D. Zhuang, H. Alradhi, Z. M. Jin, X. R. Chen, J. Shao, X. Chen, A. M. Sanchez, Y. C. Cao, J. Y. Liu, P. Yates, K. Durose, and C. J. Jin
Optically efficient InAsSb nanowires for silicon-based mid-wavelength infrared optoelectronics
Nanotechnology **28**, 105710 (2017)

Yvonne Gründer

Y. Gründer and C. A. Lucas
Probing the charge distribution at the electrochemical interface.
Phys. Chem. Chem. Phys. **19**, 8416-8422 (2017)

M. Puisto, K. Pussi, M. Alatalo, D. Hesp, V. R. Dhanak, C. A. Lucas, and Y. Gründer
LEED – IV and DFT study of the co-adsorption of chlorine and water on Cu(100)
Surf. Sci. **657**, 51-57 (2017)

Laurence Hardwick

A. Adomkevicius, L. Cabo-Fernandez, T.-H. Wu, T.-M. Ou, M.-G. Chen, Y. Andreev, C.-C. Hu, and L. J. Hardwick
$Na_{0.35}MnO_2$ as an ionic conductor with randomly distributed nano-sized layers
J. Mater. Chem. A **5**, 10021-10026 (2017)

N. E. Drewett, I. M. Aldous, J. Zou, and L. J. Hardwick
In situ Raman spectroscopic analysis of the lithiation and sodiation of antimony microparticles
Electrochimica Acta **247**, 296-305 (2017)

T. A. Galloway, L. Cabo-Fernandez, I. M. Aldous, F. Braga, and L. J. Hardwick
Shell isolated nanoparticles for enhanced Raman spectroscopy studies in lithium-oxygen cells
Faraday discuss. **205**, 469-490 (2017)

P. M. Radjenovic and L. J. Hardwick
Time-resolved SERS study of the oxygen reduction reaction in ionic liquid electrolytes for non-aqueous lithium-oxygen cells
Faraday discuss. **206**, 379-392 (2018)

M. Serwar, U. A. Rana, H. M. Siddiqi, S. Ud-Din Khan, F. A. Ahmed Ali, A. Al-Fatesh, A. Adomkevicius, J. A. Coca-Clemente, L. Cabo-Fernandez, F. Braga and L. J. Hardwick
Template-free synthesis of nitrogen doped carbon materials from an organic ionic dye (murexide) for supercapacitor application
RSC Advances **7**, 54626-54637 (2017)

J. P. Vivek, N. G. Berry, J. Zou, R. J. Nichols, and L. J. Hardwick
In Situ Surface-Enhanced Infrared Spectroscopy to Identify Oxygen Reduction Products in Nonaqueous Metal-Oxygen Batteries
J. Phys. Chem. C **121**, 19657-19667 (2017)

Frank Jäckel

J. R. Lee, W. Li, A. J. Cowan, and F. Jäckel
Hydrophilic, Hole-Delocalizing Ligand Shell to Promote Charge Transfer from Colloidal CdSe Quantum Dots in Water.
J. Phys. Chem. C **121**, 15160-15168 (2017)

Tony Lopez-Sanchez

J. Almeida, L. Da Vià, P. D. Carà, Y. Carvalho, P. N. Romano, J. A. O. Peña, L. Smith, E. F. Sousa-Aguiar, and J. A. Lopez-Sanchez
Screening of mono-and bi-functional catalysts for the one-pot conversion of cellobiose into sorbitol
Catalysis Today **279**, 187-193 (2017)

Y. Carvalho, J. Almeida, P. N. Romano, K. Farrance, P. D. Carà, N. Pereira, J. A. Lopez-Sanchez, and E. F. Sousa-Aguiar
Nanosilicalites as Support for ß-Glucosidases Covalent Immobilization
Applied Biochemistry and Biotechnology **182**, 1619-1629 (2017)

K. Lokesh, C. West, J. Kuylenstierna, J. Fan, V. Budarin, P. Priecel, J. A. Lopez-Sanchez, and J. Clark
Environmental impact assessment of wheat straw based alkyl polyglucosides produced using novel chemical approaches
Green Chemistry **19**, 4380-4395 (2017)

M. Lomelí-Rodríguez, M. Rivera-Toledo, and J. A. Lopez-Sanchez
Optimum batch-reactor operation for the synthesis of biomass-derived renewable polyesters
Ind. Eng. Chem. Res. **56**, 549-559 (2017)

M. Lomelí-Rodríguez, M. Rivera-Toledo, and J. A. Lopez-Sanchez
Process intensification of the synthesis of biomass-derived renewable polyesters: Reactive distillation and divided wall column polyesterification
Ind. Eng. Chem. Res. **56**, 3017-3032 (2017)

R. H. Padilla, P. Priecel, M. Lin, J. A. Lopez-Sanchez, and Z. Zhong
A versatile sonication-assisted deposition-reduction method for preparing supported metal catalysts for catalytic applications
Ultrasonics sonochemistry **35**, 631-639 (2017)

K. Saeed, P. Priecel, and J. A. Lopez-Sanchez
Catalytic routes towards bio-renewable glucaric acid
Chimica Oggi/Chemistry Today **35**, 7-11 (2017)

P. D. Vaidya and J. A. Lopez-Sanchez
Review of Hydrogen Production by Catalytic Aqueous-Phase Reforming
Chemistry Select **2**, 6563-6576 (2017)

L. Da Vià, C. Recchi, E. O. Gonzalez-Yañez, T. E. Davies, and J. A. Lopez-Sanchez
Visible light selective photocatalytic conversion of glucose by TiO_2
Appl. Catal. B **202**, 281-288 (2017)

Jon Major

J. D. Major, L. J. Phillips, M. Al Turkestani, L. Bowen, T. J. Whittles, V. R. Dhanak, and K. Durose
P3HT as a pinhole blocking back contact for CdTe thin film solar cells
Sol. Energy Mater. Sol. Cells **172**, 1-10 (2017)

J. D. Major, R. Tena-Zaera, E. Azaceta, L. Bowen, and K. Durose
Development of ZnO nanowire based CdTe thin film solar cells
Sol. Energy Mater. Sol. Cells **160**, 107-115 (2017)

X. Xiong, M. Forster, J. D. Major, Y. Xu, and A. J. Cowan
Time-Resolved Spectroscopy of ZnTe Photocathodes for Solar Fuel Production
J. Phys. Chem. C **121**, 22073-22080 (2017)

Alexey Sergeev

M. Jakoobi, N. Halcovitch, G. F. S. Whitehead, and A. G. Sergeev
Selective Arene Cleavage by Direct Insertion of Iridium into the Aromatic Ring
Angew. Chem. Int. Ed. **56**, 3266-3269 (2017)

Dmitry Shchukin

M. Graham, J. A. Coca-Clemente, E. Shchukina, and D. Shchukin
Nanoencapsulated crystallohydrate mixtures for advanced thermal energy storage
J. Mater. Chem. A **5**, 13683-13691 (2017)

D. Grigoriev, E. Shchukina, and D. G. Shchukin
Nanocontainers for Self-Healing Coatings
Adv. Mater. Interfaces **4**, 201600318 (2017)

G. Li, J. Hu, H. Wang, C. Pilz-Allen, J. Wang, T. Qi, H. Möhwald, D. G. Shchukin
Polymer-decorated Anisotropic Silica Nanotubes with Combined Shape and Surface Properties for Guest Delivery
Polymer, **109**, 332-338 (2017)

L. Martín-Olivera, D. G. Shchukin, and G. Teobaldi
Role of Metal Lattice Expansion and Molecular π-Conjugation for the Magnetic Hardening at Cu-Organics Interfaces
J. Phys. Chem. C **121**, 23777-23787 (2017)

M. Michailidis, I. Sorzabal-Bellido, E. A. Adamidou, Y. A. Diaz-Fernandez, J. Aveyard, R. Wengier, D. Grigoriev, R. Raval, Y. Benayahu, R. A. D'Sa, and D. Shchukin
Modified Mesoporous Silica Nanoparticles with a Dual Synergetic Antibacterial Effect
ACS Appl. Mater. Interfaces **9**, 38364-38372 (2017)

M. Oroval, C. Coll, A. Bernardos, M. D. Marcos, R. Martinez-Manez, D. G. Shchukin, and F. Sancenón
Selective Fluorogenic Sensing of As(III) Using Aptamer-Capped Nanomaterials
ACS Appl. Mater. Interfaces **9**, 11332-11336 (2017)

V. Z. Prokopovic, A. S. Vikulina, D. Sustr, E. M. Shchukina, D. G. Shchukin, and D. V. Volodkin
Binding Mechanism of the Model Charged Dye Carboxyfluorescein to Hyaluronan/Polylysine Multilayers
ACS Appl. Mater. Interfaces **9**, 38908-38918 (2017)

D. G. Shchukin, E. Shchukina
Applications of the Clay Materials as Nanocontainers for Self-Healing Coatings
In "Functional Polymer Composites with Nanoclays",
Y. Lvov, B. Guo, R. F. Fakhrullin (Eds)
Book Series: RSC Smart Materials, **22**, 223-244 (2017)

E. Shchukina, D. Grigoriev, T. Sviridova, and D. Shchukin
Comparative study of the effect of halloysite nanocontainers on autonomic corrosion protection of polyepoxy coatings on steel by salt-spray tests
Prog. Org. Coat. **108**, 84-89 (2017)

E. Shchukina, D. Shchukin, and D. Grigoriev
Effect of inhibitor-loaded halloysites and mesoporous silica nanocontainers on corrosion protection of powder coatings
Prog. Org. Coat. **102**, 60-65 (2017)

Z. Zheng, Z. Chang, G.-K. Xu, F. McBride, A. Ho, Z. Zhuola, M. Michailidis, W. Li, R. Raval, R. Akhtar and D. G. Shchukin
Microencapsulated Phase Change Materials in Solar-Thermal Conversion Systems: Understanding Geometry-Dependent Heating Efficiency and System Reliability
ACS Nano **11**, 721-729 (2017)

Gilberto Teobaldi

F. Al Ma'Mari, M. Rogers, S. Alghamdi, T. Moorsom, S. Lee, T. Prokscha, H. Luetkens, M. Valvidares, G. Teobaldi, M. Flokstra, R. Stewart, P. Gargiani, M. Ali, G. Burnell, B. J. Hickey, and O. Cespedes
Emergent magnetism at transition-metal-nanocarbon interfaces
Proc. Nat. Acad. Sci. **114**, 5583-5588 (2017)

J. D. Elliott, E. Poli, I. Scivetti, L. E. Ratcliff, L. Andrinopoulos, J. Dziedzic, N. D. M. Hine, A. A. Mostofi, C. K. Skylaris, P. D. Haynes and G. Teobaldi
Chemically Selective Alternatives to Photoferroelectrics for Polarization-Enhanced Photocatalysis: the Untapped Potential of Hybrid Inorganic Nanotubes
Adv. Sci. **4**, 1600153 (2017)

L. Martín-Olivera, D. G. Shchukin, and G. Teobaldi
Role of Metal Lattice Expansion and Molecular π-Conjugation for the Magnetic Hardening at Cu-Organics Interfaces
J. Phys. Chem. C **121**, 23777-23787 (2017)

Tim Veal

E. A. Anyebe, I. Sandall, Z. M. Jin, A. M. Sanchez, M. K. Rajpalke, T. D. Veal, Y. C. Cao, H. D. Li, R. Harvey, and Q. D. Zhuang
Optimization of self-catalyzed InAs Nanowires on flexible graphite for photovoltaic infrared photodetectors
Sci. Rep. **7**, 46110 (2017)

E. Arca, A. B. Kehoe, T. D. Veal, A. Shmeliov, D. O. Scanlon, C. Downing, D. Daly, D. Mullarkey, I. V. Shvets, V. Nicolosi, and G. W. Watson
Valence band modification of Cr_2O_3 by Ni-doping: Creating a high figure of merit p-type TCO
J. Mater. Chem. C **5**, 12610-12618 (2017)

M. Birkett, C. N. Savory, A. N. Fioretti, P. Thompson, C. A. Muryn, A. D. Weerakkody, I. Z. Mitrovic, S. Hall, R. Treharne, V. R. Dhanak, D. O. Scanlon, A. Zakutayev, and T. D. Veal
Atypically small temperature-dependence of the direct band gap in the metastable semiconductor copper nitride Cu_3N
Phys. Rev. B **95**, 115201 (2017)

W. M. Linhart, M. Gladysiewicz, J. Kopaczek, M. K. Rajpalke, M. J. Ashwin, T. D. Veal, and R. Kudrawiec
Indium-incorporation enhancement of photoluminescence properties of Ga(In)SbBi alloys
J. Phys. D.:Appl. Phys. **50**, 375102 (2017)

N. Segercrantz, J. Slotte, I. Makkonen, F. Tuomisto, I. C. Sandall, M. J. Ashwin, and T. D. Veal
Hole density and acceptor-type defects in MBE-grown $GaSb_{1-x}Bi_x$
J. Phys. D.:Appl. Phys. **50**, 295102 (2017)

T. J. Whittles, T. D. Veal, C. N. Savory, A. W. Welch, F. W. de Souza Lucas, J. T. Gibbon, M. Birkett, R. J. Potter, D. O. Scanlon, A. Zakutayev, and V. R. Dhanak
Core-Levels, Band Alignments, and Valence Band States in $CuSbS_2$ for Solar Cell Applications.
ACS Appl. Mater. Interfaces **9**, 41916-41926 (2017)

Publications by SIRE academic staff in 2018

Jonathan Alaria

M. Birkett, W. M. Linhart, J. Stoner, L. J. Phillips, K. Durose, J. Alaria, J. D. Major, R. Kudrawiec and T. D. Veal
Band gap temperature-dependence of close-space sublimation grown Sb_2Se_3 by photo-reflectance
APL Mater. **6**, 084901 (2018)

L. M. Daniels, S. Ling, S. N. Savvin, M. J. Pitcher, M. S. Dyer, J. B. Claridge, B. Slater, F. Corà, J. Alaria and M. J. Rosseinsky
A and B site doping of a phonon-glass perovskite oxide thermoelectric
J. Mater. Chem. A **6**, 15640-15652 (2018).

C. Delacotte, G. F. S. Whitehead, M. J. Pitcher, C. M. Robertson, P. M. Sharp, M. S. Dyer, J. Alaria, J. B. Claridge, G. R. Darling, D. R. Allan, G. Winter, and M. J. Rosseinsky
Structure determination and crystal chemistry of large repeat mixed-layer hexaferrites
IUCRJ **5**, 681-698 (2018)

Q. D. Gibson, M. S. Dyer, C. Robertson, C. Delacotte, T. D. Manning, M. J. Pitcher, L. M. Daniels, M. Zanella, J. Alaria, J. B. Claridge, and M. J. Rosseinsky
$Bi_{2+2n}O_{2+2n}Cu_{2-\delta}Se_{2+n-\delta}X_\delta$ (X = Cl, Br): A Three-Anion Homologous Series
Inorganic Chemistry **57**, 12489-12500 (2018)

C. A. Tzitzeklis, J. K. Gupta, M. S. Dyer, T. D. Manning, M. J. Pitcher, H. J. Niu, S. Savvin, J. Alaria, G. R. Darling, J. B. Claridge, and M. J. Rosseinsky
Computational Prediction and Experimental Realization of p-Type Carriers in the Wide-Band-Gap Oxide $SrZn_{1-x}Li_xO_2$
Inorganic Chemistry **57**, 11874-11883 (2018)

Frédéric Blanc

F. Blanc
CdSe Semiconductor Nanocrystals: The Surface and the Core.
ACS Central Science **4**, 1081-1083 (2018)

N. J. Brownbill, R. S. Sprick, B. Bonillo, S. Pawsey, F. Aussenac, A. J. Fielding, A. I. Cooper, and F. Blanc
Structural Elucidation of Amorphous Photocatalytic Polymers from Dynamic Nuclear Polarization Enhanced Solid State NMR
Macromolecules **51**, 3088-3096 (2018)

L. Buannic, L. Sperrin, R. Dervisoglu, F. Blanc, and C. P. Grey
Proton distribution in Sc-doped $BaZrO_3$: a solid state NMR and first principle calculations analysis
Phys. Chem. Chem. Phys. **20**, 4317-4328 (2018)

M. Craven, D. Xiao, C. Kunstmann-Olsen, E. F. Kozhevnikova, F. Blanc, A. Steiner, and I. V. Kozhevnikov
Oxidative desulfurization of diesel fuel catalyzed by polyoxometalate immobilized on phosphazene-functionalized silica
Appl. Catal. B **231**, 82-91 (2018)

B. Dong, J. Yan, B. Walkley, K. K. Inglis, F. Blanc, S. Hull, and A. R. West
Synthesis and characterisation of the new oxyfluoride Li^+ ion conductor Li_5SiO_4F
Solid State Ionics **327**, 64-70 (2018)

A. Fernandes, R. F. Moran, S. Sneddon, D. M. Dawson, D. McKay, G. P. M. Bignami, F. Blanc, K. R. Whittle, and S. E. Ashbrook
^{17}O solid-state NMR spectroscopy of $A_2B_2O_7$ oxides: quantitative isotopic enrichment and spectral acquisition?
RSC Advances **8**, 7089-7101 (2018)

K. Jie, M. Liu, Y. Zhou, M. A. Little, A. Pulido, S. Y. Chong, A. Stephenson, A. R. Hughes, F. Sakakibara, T. Ogoshi, F. Blanc, G. M. Day, F. Huang, and A. I. Cooper
Near-Ideal Xylene Selectivity in Adaptive Molecular Pillar[n]arene Crystals
J. Am. Chem. Soc. **140**, 6921-6930 (2018)

B. T. Leube, K. K. Inglis, E. J. Carrington, P. M. Sharp, J. F. Shin, A. R. Neale, T. R. Manning, M. J. Pitcher, L. J. Hardwick, M. S, Dyer, F. Blanc, J. B. Claridge, and M. J. Rosseinsky
Lithium Transport in $Li_{4.4}M_{0.4}M'_{0.6}S_4$ (M = Al^{3+}, Ga^{3+}, and M' = Ge^{4+}, Sn^{4+}): Combined Crystallographic, Conductivity, Solid State NMR, and Computational Studies
Chem. Mater. **30**, 7183-7200 (2018)

L. Longley, S. M. Collins, C. Zhou, G. J. Smales, S. E. Norman, N. J. Brownbill, C. W. Ashling, P. A. Chater, R. Tovey, C.-B. Schönlieb, T. F. Headen, N. J. Terrill, Y. Yue, A. J. Smith, F. Blanc, D. A. Keen, P. A. Midgley, and T. D. Bennett
Liquid phase blending of metal-organic frameworks
Nat. Commun. **9**, 2135 (2018)

M. Sachs, R. S. Sprick, D. Pearce, S. A. J. Hillman, A. Monti, A. A. Y. Guilbert, N. J. Brownbill, S. Dimitrov, X. Shi, F. Blanc, M. A. Zwijnenburg, J. Nelson, J. R. Durrant and A. I. Cooper
Understanding structure-activity relationships in linear polymer photocatalysts for hydrogen evolution
Nat. Commun. **9**, 4968 (2018)

D. Xiao, S. Xu, N. J. Brownbill, S. Paul, L.-H. Chen, S. Pawsey, F. Aussenac, B.-L. Su, X. Han, X. Bao, Z. Liu and F. Blanc
Fast detection and structural identification of carbocations on zeolites by dynamic nuclear polarization enhanced solid-state NMR
Chemical Science **9**, 8184-8193 (2018)

Alex Cowan

A. J. Cowan
Surface-selective and Time-resolved Spectro-electrochemical Studies of CO_2 Reduction Mechanisms Chapter 10 in F. Marken and D. Fermin (Eds), RSC Energy and Environment Series No. 21, pp. 244-263 (Royal Society of Chemistry, Cambridge, 2018)

M. Forster, R. Potter, Y. Yang, Y. Li, and A. J. Cowan
Stable Ta_2O_5 overlayers on α-Fe_2O_3 can enhance photoelectrochemical water splitting efficiencies
ChemPhotoChem **2**, 183-189 (2018)

M. F. Kuehnel, C. D. Sahm, G. Neri, J. R. Lee, K. L. Orchard, A. J. Cowan, and E. Reisner
ZnSe quantum dots modified with a Ni(cyclam) catalyst for efficient visible-light driven CO_2 reduction in water
Chemical Science **9**, 2501-2509 (2018)

G. Neri, M. Forster, and A. J. Cowan,
Photochemical Energy Storage
Chapter 5 in R. E. Hester and R. M. Harrison (Eds), Energy Storage Options and Their Environmental Impact, pp. 184-209 (Royal Society of Chemistry, Cambridge, 2018)

G. Neri, J. J. Walsh, G. Teobaldi, P. M. Donaldson, and A. J. Cowan
Detection of catalytic intermediates at an electrode surface during carbon dioxide reduction by an earth-abundant catalyst
Nature Catalysis **1**, 952-959 (2018)

J. J. Walsh, M. Forster, C. L. Smith, G. Neri, R. J. Potter, and A. J. Cowan
Directing the mechanism of CO_2 reduction by a Mn catalyst through surface immobilization. Phys. Chem. Chem. Phys. **20**, 6811-6816 (2018)

Vin Dhanak

J. T. Gibbon, L. Jones, J. W. Roberts, M. Althobaiti, P. R. Chalker, I. Z. Mitrovic, and V. R. Dhanak
Band alignments at Ga_2O_3 heterojunction interfaces with Si and Ge
AIP Advances **8**, 065011 (2018)

M. Mattinen, P. J. King, L. Khriachtchev, K. Meinander, J. T. Gibbon, V. R. Dhanak, J. Räisänen, M. Ritala, and M. Leskelä
Low-Temperature Wafer-Scale Deposition of Continuous 2D SnS_2 Films.

Small **14**, 1800547 (2018)

I. Z. Mitrovic, A. D. Weerakkody, N. Sedghi, J. F. Ralph, S. Hall, V. R. Dhanak, Z. Luo, and S. Beeby
Controlled modification of resonant tunneling in metal-insulator-insulator-metal structures
Appl. Phys. Lett. **112**, 012902 (2018)

J. E. N. Swallow, B. A. D. Williamson, M. Birkett, A. Abbott, M. Farnworth, T. J. Featherstone, N. Peng, K. J. Cheetham, P. Warren, A. Regoutz, D. A. Duncan, T.-L. Lee, D. O. Scanlon, V. R. Dhanak, and T. D. Veal
A hard X-ray photoemission study of transparent conducting fluorine-doped tin dioxide
In 2018 IEEE 7th World Conference on Photovoltaic Energy Conversion, WCPEC 2018 – A Joint Conference of 45th IEEE PVSC, 28th PVSEC and 34th EU PVSEC (pp. 3051-3055)

J. E. N. Swallow, B. A. D. Williamson, T. J. Whittles, M. Birkett, T. J. Featherstone, N. Peng, A. Abbott, M. Farnworth, K. J. Cheetham, P. Warren, D. O. Scanlon, V. R. Dhanak, and T. D. Veal
Self-compensation in transparent conducting F-doped SnO_2
Adv. Funct. Mater. **28**, 1701900 (2018)

J. Y. Zhang, W. W. Li, R. L. Z. Hoye, J. L. MacManus-Driscoll, M. Budde, O. Bierwagen, L. Wang, Y. Du, M. J. Wahila, L. F. J. Piper, T.-L. Lee, H. J. Edwards, V. R. Dhanak, and K. H. L. Zhang
Electronic and transport properties of Li-doped NiO epitaxial thin films
J. Mater. Chem. C **6**, 2275-2282 (2018)

L. Žurauskaite, L. Jones, V. R. Dhanak, I. Z. Mitrovic, P. E. Hellström, and M. Östling
Investigation of Tm_2O_3 as a gate dielectric for Ge MOS devices
ECS Trans. **86**, 67-73 (2018)

Ken Durose

T. Baines, K. Durose, and J. D. Major
Co-Sputtered $Mg_xZn_{(1-x)}O$ window layers for $CdTe_{(1-x)}Se_x$ solar cells
In 2018 IEEE 7th World Conference on Photovoltaic Energy Conversion, WCPEC 2018 – A Joint Conference of 45th IEEE PVSC, 28th PVSEC and 34th EU PVSEC (pp. 2974-2979)

T. Baines, G. Papageorgiou, O. S. Hutter, L. Bowen, K. Durose, and J. D. Major
Self-Catalyzed CdTe Wires Nanomaterials **8**, 274 (2018)

T. Baines, G. Zoppi, L. Bowen, T. P. Shalvey, S. Mariotti, K. Durose, and J. D. Major
Incorporation of CdSe layers into CdTe thin film solar cells
Sol. Energy Mater. Sol. Cells **180**, 196-204 (2018)

M. Birkett, W. M. Linhart, J. Stoner, L. J. Phillips, K. Durose, J. Alaria, J. D. Major, R. Kudrawiec, and T. D. Veal,
Band gap temperature-dependence of close-space sublimation grown Sb_2Se_3 by photo-reflectance
APL Mater. **6**, 084901 (2018)

T. J. Featherstone, J. E. N. Swallow, J. D. Major, K. Durose, and T. D. Veal
Transparent Ta doped SnO_2 films deposited by RF co-sputtering
In 2018 IEEE 7th World Conference on Photovoltaic Energy Conversion, WCPEC 2018 – A Joint Conference of 45th IEEE PVSC, 28th PVSEC and 34th EU PVSEC (pp. 2980-2984)

T. D. C. Hobson, O. S. Hutter, M. Birkett, T. D. Veal, and K. Durose
Growth and Characterization of Sb_2Se_3 Single Crystals for Fundamental Studies
In 2018 IEEE 7th World Conference on Photovoltaic Energy Conversion, WCPEC 2018 – A Joint Conference of 45th IEEE PVSC, 28th PVSEC and 34th EU PVSEC (pp. 818-822)

O. S. Hutter, L. J. Phillips, K. Durose, and J. D. Major
6.6% efficient antimony selenide solar cells using grain structure control and an organic contact layer
Sol. Energy. Mat. Sol. Cells **188**, 177-181 (2018)

O. S. Hutter, L. J. Phillips, P. J. Yates, J. D. Major, and K. Durose
CSS Antimony Selenide Film Morphology and High Efficiency PV Devices
In 2018 IEEE 7th World Conference on Photovoltaic Energy Conversion, WCPEC 2018 – A Joint Conference of 45th IEEE PVSC, 28th PVSEC and 34th EU PVSEC (pp. 27-31)

S. Mariotti, O. S. Hutter, L. J. Phillips, P. J. Yates, B. Kundu, and K. Durose
Stability and Performance of $CsPbI_2Br$ Thin Films and Solar Cell Devices
ACS Appl. Mater. Interfaces **10**, 3750-3760 (2018)

L. J. Phillips, C. N. Savory, O. S. Hutter, P. J. Yates, H. Shiel, S. Mariotti, L. Bowen, M. Birkett, K. Durose, D. O. Scanlon, and J. D. Major
Current enhancement via a TiO_2 window layer for CSS Sb_2Se_3 solar cells: performance limits and high V_{oc}
IEEE J. Photovoltaics **9**, 544-551 (2018)

T. P. Shalvey, L. J. Phillips, K. Durose, and J. D. Major
A comparison of organic back contact materials for CdTe solar cells
In 2018 IEEE 7th World Conference on Photovoltaic Energy Conversion, WCPEC 2018 – A Joint Conference of 45th IEEE PVSC, 28th PVSEC and 34th EU PVSEC (pp. 846-851)

Yvonne Gründer

Y. Gründer, J. Stettner, and O. M. Magnussen
Review: In-Situ Surface X-ray Diffraction Studies of Copper Electrodes: Atomic-Scale Interface Structure and Growth Behavior
J. Electrochem. Soc. **166**, D3049-D3057 (2018)

Y. Joly, A. Abisset, A. Bailly, M. De Santis, F. Fettar, S. Grenier, D. Mannix, A. Y. Ramos, M.-C. Saint-Lager, Y. Soldo-Olivier, J.-M. Tonnerre, S. A. Guda, and Y. Gründer
Simulation of Surface Resonant X-ray Diffraction
J. Chem. Theory Comput. **14**, 973-980 (2018)

Laurence Hardwick

M. Addicoat, R. Atkin, J. N. C. Lopes, M. C. Gomes, M. Firestone, R. Gardas, S. Halstead, C. Hardacre, L. J. Hardwick, J. Holbrey, P. Hunt, V. Ivaništšev, J. Jacquemin, R. Jones, B. Kirchner, R. Lynden-Bell, D. MacFarlane, G. Marlair, H. Medhi, M. Mezger, A. Pádua, I. Pantenburg, S. Perkin, J. E. S. J. Reid, M. Rutland, S. Saha, K. Shimizu, J. M. Slattery, M. Swadźba-Kwaśny, S. Tiwari, S. Tsuzuki, B. Uralcan, A. van den Bruinhorst, M. Watanabe, and J. Wishart
Structure and dynamics of ionic liquids: general discussion.
Faraday Discussions **206**, 291-337 (2018)

I. M. Aldous and L. J. Hardwick
Growth and dissolution of NaO_2 in an ether-based electrolyte as the discharge product in the Na-O_2 cell
Chem. Comm. **54**, 3444-3447 (2018)

L. J. Hardwick and C. P. de Leon
Rechargeable Multi-Valent Metal-Air Batteries: A review of research and current challenges in secondary multivalent metal-oxygen batteries
Johnson Matthey Technology Review **62**, 134-149 (2018)

B. T. Leube, K. K. Inglis, E. J. Carrington, P. M. Sharp, J. F. Shin, A. R. Neale, T. R. Manning, M. J. Pitcher, L. J. Hardwick, M. S. Dyer, F. Blanc, J. B. Claridge, and M. J. Rosseinsky
Lithium Transport in $Li_{4.4}M_{0.4}M'_{0.6}S4$ ($M = Al^{3+}$, Ga^{3+}, and $M' = Ge^{4+}$, Sn^{4+}): Combined Crystallographic, Conductivity, Solid State NMR, and Computational Studies
Chem. Mater. **30**, 7183-7200 (2018)

P. M. Radjenovic and L. J. Hardwick
Time-resolved SERS study of the oxygen reduction reaction in ionic liquid electrolytes for non-aqueous lithium-oxygen cells
Faraday Discussions **206**, 379-392 (2018)

Frank Jäckel

W. Li and F. Jäckel
Size-controlled electron transfer rates determine hydrogen generation efficiency in colloidal Pt-decorated CdS quantum dots
Nanoscale **10**, 16153-16158 (2018)

C. M. Wolff, P. D. Frischmann, M. Schulze, B. J. Bohn, R. Wein, P. Livadas, M. T. Carlson, F. Jäckel, J. Feldmann, F. Würthner, and J. K. Stolarczyk
All-in-one visible-light-driven water splitting by combining nanoparticulate and molecular co-catalysts on CdS nanorods
Nature Energy **3**, 862-869 (2018)

Tony Lopez-Sanchez

S. Christy, A. Noschese, M. Lomelí-Rodriguez, N. Greeves, and J. A. Lopez-Sanchez
Recent progress in the synthesis and applications of glycerol carbonate
Curr. Opin. Green Sustain. Chem. **14**, 99-107 (2018)

M. Lomeli-Rodriguez, J. R. Corpas-Martinez, S. Willis, R. Mulholland, and J. A. Lopez-Sanchez
Synthesis and Characterization of Renewable Polyester Coil Coatings from Biomass-Derived Isosorbide, FDCA, 1,5-Pentanediol, Succinic Acid, and 1,3-Propanediol
Polymers **10**, 600 (2018)

J. McGlone, P. Priecel, L. Da Via, L. Majdal, and J. A. Lopez-Sanchez

Desilicated ZSM-5 Zeolites for the Production of Renewable p-Xylene via Diels-Alder Cycloaddition of Dimethylfuran and Ethylene
Catalysts **8**, 253 (2018)

P. Priecel, N. A. Endot, P. D. Carà, and J. A. Lopez-Sanchez
Fast Catalytic Hydrogenation of 2,5-Hydroxymethylfurfural to 2,5-Dimethylfuran with Ruthenium on Carbon Nanotubes
Ind. Eng. Chem. Res. **57**, 1991-2002 (2018)

P. Priecel, J. E. Perez Mejia, P. D. Carà, and J. A. Lopez-Sanchez
Microwaves in the Catalytic Valorisation of Biomass Derivatives
Chapter 8 in G. A. Kraus, A. Stankiewicz, and P. Siedl (Eds), RSC Green Chemistry No. 56, pp. 243-299 (Royal Society of Chemistry, Cambridge, 2018)

Jon Major

T. Baines, K. Durose, and J. D. Major
Co-Sputtered $Mg_xZn_{(1-x)}O$ window layers for $CdTe_{(1-x)}Se_x$ solar cells
In 2018 IEEE 7th World Conference on Photovoltaic Energy Conversion, WCPEC 2018 – A Joint Conference of 45th IEEE PVSC, 28th PVSEC and 34th EU PVSEC (pp. 2974-2979)

T. Baines, G. Papageorgiou, O. S. Hutter, L. Bowen, K. Durose, and J. D. Major
Self-Catalyzed CdTe Wires
Nanomaterials **8**, 274 (2018)

T. Baines, G. Zoppi, L. Bowen, T. P. Shalvey, S. Mariotti, K. Durose, and J. D. Major
Incorporation of CdSe layers into CdTe thin film solar cells
Sol. Energy Mater. Sol. Cells **180**, 196-204 (2018)

M. Birkett, W. M. Linhart, J. Stoner, L. J. Phillips, K. Durose, J. Alaria, J. D. Major, R. Kudrawiec, and T. D. Veal,
Band gap temperature-dependence of close-space sublimation grown Sb_2Se_3 by photo-reflectance
APL Mater. **6**, 084901 (2018)

T. J. Featherstone, J. E. N. Swallow, J. D. Major, K. Durose, and T. D. Veal
Transparent Ta doped SnO_2 films deposited by RF co-sputtering
In 2018 IEEE 7th World Conference on Photovoltaic Energy Conversion, WCPEC 2018 – A Joint Conference of 45th IEEE PVSC, 28th PVSEC and 34th EU PVSEC (pp. 2980-2984)

T. D. C. Hobson, O. S. Hutter, M. Birkett, T. D. Veal, and K. Durose
Growth and Characterization of Sb_2Se_3 Single Crystals for Fundamental Studies
In 2018 IEEE 7th World Conference on Photovoltaic Energy Conversion, WCPEC 2018 – A Joint Conference of 45th IEEE PVSC, 28th PVSEC and 34th EU PVSEC (pp. 818-822)

O. S. Hutter, L. J. Phillips, K. Durose, and J. D. Major
6.6% efficient antimony selenide solar cells using grain structure control and an organic contact layer
Sol. Energy. Mat. Sol. Cells **188**, 177-181 (2018)

O. S. Hutter, L. J. Phillips, P. J. Yates, J. D. Major, and K. Durose
CSS Antimony Selenide Film Morphology and High Efficiency PV Devices
In 2018 IEEE 7th World Conference on Photovoltaic Energy Conversion, WCPEC 2018 – A Joint Conference of 45th IEEE PVSC, 28th PVSEC and 34th EU PVSEC (pp. 27-31)

L. J. Phillips, C. N. Savory, O. S. Hutter, P. J. Yates, H. Shiel, S. Mariotti, L. Bowen, M. Birkett, K. Durose, D. O. Scanlon, and J. D. Major
Current enhancement via a TiO_2 window layer for CSS Sb_2Se_3 solar cells: performance limits and high V_{oc}
IEEE J. Photovoltaics **9**, 544-551 (2018)

T. P. Shalvey, L. J. Phillips, K. Durose, and J. D. Major
A comparison of organic back contact materials for CdTe solar cells
In 2018 IEEE 7th World Conference on Photovoltaic Energy Conversion, WCPEC 2018 – A Joint Conference of 45th IEEE PVSC, 28th PVSEC and 34th EU PVSEC (pp. 846-851)

Dmitry Shchukin

E. M. Shchukina, M. Graham, Z. Zheng, and D. G. Shchukin
Nanoencapsulation of phase change materials for advanced thermal energy storage systems
Chem. Soc. Rev. **47**, 4156-4175 (2018)

H. Wei, D. G. Shchukin, and C. Li,
Study on the capacity of mesoporous alumina with different pore sizes absorb silane inhibitors
Surf. Interface Anal. **50**, 688-695 (2018)

Q. Ye, J. Zhang, P. Guo, H. Fan, D. Shchukin, B. Wei, and H. Wang
Wet-Chemical Synthesis of Surface-Passivated Halide Perovskite Microwires for Improved Optoelectronic Performance and Stability
ACS Appl. Mater. Interfaces **10**, 43850-43856 (2018)

Tim Veal

M. Birkett, W. M. Linhart, J. Stoner, L. J. Phillips, K. Durose, J. Alaria, J. D. Major, R. Kudrawiec, and T. D. Veal
Band gap temperature-dependence of close-space sublimation grown Sb_2Se_3 by photo-reflectance APL Mater. **6**, 084901 (2018)

M. Birkett, C. N. Savory, M. K. Rajpalke, W. M. Linhart, T. J. Whittles, J. T. Gibbon, A. W. Welch, I. Z. Mitrovic, A. Zakutayev, D. O. Scanlon, and T. D. Veal
Band gap temperature-dependence and exciton-like state in copper antimony sulphide, $CuSbS_2$
APL Mater. **6**, 084904 (2018)

T. J. Featherstone, J. E. N. Swallow, J. D. Major, K. Durose, and T. D. Veal
Transparent Ta doped SnO_2 films deposited by RF co-sputtering
In 2018 IEEE 7th World Conference on Photovoltaic Energy Conversion, WCPEC 2018 – A Joint Conference of 45th IEEE PVSC, 28th PVSEC and 34th EU PVSEC (pp. 2980-2984)

T. D. C. Hobson, O. S. Hutter, M. Birkett, T. D. Veal, and K. Durose
Growth and Characterization of Sb_2Se_3 Single Crystals for Fundamental Studies
In 2018 IEEE 7th World Conference on Photovoltaic Energy Conversion, WCPEC 2018 – A Joint Conference of 45th IEEE PVSC, 28th PVSEC and 34th EU PVSEC (pp. 818-822)

J. E. N. Swallow, B. A. D. Williamson, M. Birkett, A. Abbott, M. Farnworth, T. J. Featherstone, N. Peng, K. J. Cheetham, P. Warren, A. Regoutz, D. A. Duncan, T.-L. Lee, D. O. Scanlon, V. R. Dhanak, and T. D. Veal
A hard X-ray photoemission study of transparent conducting fluorine-doped tin dioxide
In 2018 IEEE 7th World Conference on Photovoltaic Energy Conversion, WCPEC 2018 – A Joint Conference of 45th IEEE PVSC, 28th PVSEC and 34th EU PVSEC (pp. 3051-3055)

J. E. N. Swallow, B. A. D. Williamson, T. J. Whittles, M. Birkett, T. J. Featherstone, N. Peng, A. Abbott, M. Farnworth, K. J. Cheetham, P. Warren, D. O. Scanlon, V. R. Dhanak, and T. D. Veal
Self-compensation in transparent conducting F-doped SnO_2
Adv. Funct. Mater. **28**, 1701900 (2018)

Research Grants Held in 2017

SIRE hold more than £21,000,000 in active grants.
New grants won in 2017 are marked with an asterisk.

Engineering & Physical Sciences Research Council

*J. Alaria, Layered oxide thermoelectrics for high temperature waste heat recovery,	**£100,579**
F. Blanc, Dynamic nuclear polarization solid-state nuclear magnetic resonance spectroscopy of intensive nuclear spins,	**£60,624**
A. J. Cowan, Spectroscopy-driven design of an efficient photocatalyst for CO_2 reduction,	**£885,066**
A. J. Cowan, Spectroscopy-driven design of an efficient photocatalyst for CO_2 reduction, Fellowship Extension,	**£627,696**
A. J. Cowan, M. J. Rosseinsky (PI) et al., £1.8M, Flexible Routes to Liquid Fuels from CO_2 by Advanced Catalysis and Engineering,	**£1,804,265**
*V. R. Dhanak, Peter Weightman (PI), and Michele Siggel-King, FLUENCE,	**£630,891**
K. Durose, Improved Understanding, Development and Optimisation of Perovskite-based Solar Cells,	**£93,490**
K. Durose, EPSRC Centre for Doctoral Training in New and Sustainable Photovoltaics,	**£5,260,808**
K. Durose, SUPERSOLAR Solar Energy Hub,	**£337,851**
*K. Durose, SUPERSOLAR flexible funding-planar Heterojunctions for perovskite-based PV: optical design, heterostructure screening and junction properties,	**£120,237**
K. Durose, EPSRC Centre for Doctoral Training in New and Sustainable Photovoltaics, Equipment account,	**£280,000**
K. Durose, Overcoming the grain size limit to V_{oc} in sustainable photovoltaics,	**£508,351**
*L. J. Hardwick, The Calcium-Air Battery,	**£251,028**
*L. J. Hardwick, ISCF Wave 1: Earth-Abundant Metal-Air Batteries,	**£909,900**
*L. J. Hardwick and A. I. Cooper (PI), Porous Liquids: Understanding, Scope and Applications,	**£535,720**
L. J. Hardwick, Growth and dissolution mechanism of metal oxides in metal-air batteries,	**£95,557**
L. J. Hardwick, Multi-scale analysis for facilities for energy storage (manifest),	**£89,274**
L. J. Hardwick, The role of electrocatalysts in the oxygen reduction reaction in non-aqueous electrolytes,	**£354,296**
L. J Hardwick, Electrochemical energy storage with graphene-enabled materials,	**£642,250**
F. Jäckel, R. Nichols (PI), S. Higgins, Single-Molecule Plasmoelectronics,	**£444,776**
J. A. Lopez-Sanchez, Renewable chemicals from sustainable feedstocks via high-throughput methods,	**£1,042,294**
J. A. Lopez-Sanchez, Bio-renewable formulation information and knowledge management system,	**£20,167**
*J. D. Major, Capacitance spectroscopy led process innovations to improve V_{OC} in CdTe thin film solar cells,	**£810,101**
T. D. Veal, V. R. Dhanak, Donor design for maximum mobility transparent conducting oxides,	**£509,182**

European Commission

A. J. Cowan, SEAFUEL – Sustainable integration of renewable fuels in local transportation (Interreg Atlantic area (ERDF)),	**£187,000**
K. Durose, NanoEmbrace – Embracing one dimensional semiconductor nanostructures,	**£233,886**
*K. Durose, INDEED, Innovative Nanowire DEvicE Design, Marie Curie European Training Network,	**£308,208**
*D. Shchukin, ERC Proof-of-Concept award ENERPAINT,	**£130,000**
D. Shchukin, NonaBarrier – Extended shelf-life biopolymers for sustainable and multifunctional food packaging solutions	**£420,952**
D. Shchukin, BYEFOULING – Low-toxic cost-efficient environment-friendly antifouling materials,	**£290,000**
D. Shchukin, SONO ENGINEERING – Electronic structures sono-engineering of semiconductor nanoparticle for efficient solar energy exploitation,	**£185,340**
D. Shchukin, ENERCAPSULE – Nanoencapsulation for energy storage and controlled release,	**£1,594,670**

Industry

*F. Blanc, Bristol-Myers Squibb, Amorphous Solid Dispersion,	**£40,000**
L. J. Hardwick, Johnson Matthey, In situ Raman and IR studies for Lithium Battery Materials,	**£30,000**
*T. D. Veal, V. R. Dhanak and J. D. Major, NSG Group (Pilkington), Band alignments in inorganic thin film solar cells and transparent conductors,	**£12,000**

Innovate (UK)

*L. J. Hardwick, Practical lithium air batteries,	**£95,087**
*L. J. Hardwick, Practical and Robust Lithium Air Batteries,	**£137,300**
*D. Shchukin, Innovative Assembly Processes and Equipment for Healthier Foods' Emulsions and New Market Opportunities (together with Unilever),	**£980,000**

NATO

*D. Shchukin, NATO Science for Peace project "Functional Textiles for Uniforms" (together with University of Georgia, USA),	**£310,000**

Royal Society

F. Blanc, Spectroscopic structural investigation of La doped $SrTiO_3$ anodes,	**£24,000**
Y. Gründer, Electrochemistry in non-aqueous solvents,	**£134,337**
L. J. Hardwick, Understanding the Oxygen Reduction and Evolution Reaction Using SHINERS,	**£12,000**
A. Sergeev, Selective reduction of arenes to alkanes by assisted tandem catalysis,	**£14,807**
G. Teobaldi, Advanced new linear-scaling constrained density-functional theory approaches,	**£11,995**

Science and Technology Facilities Council

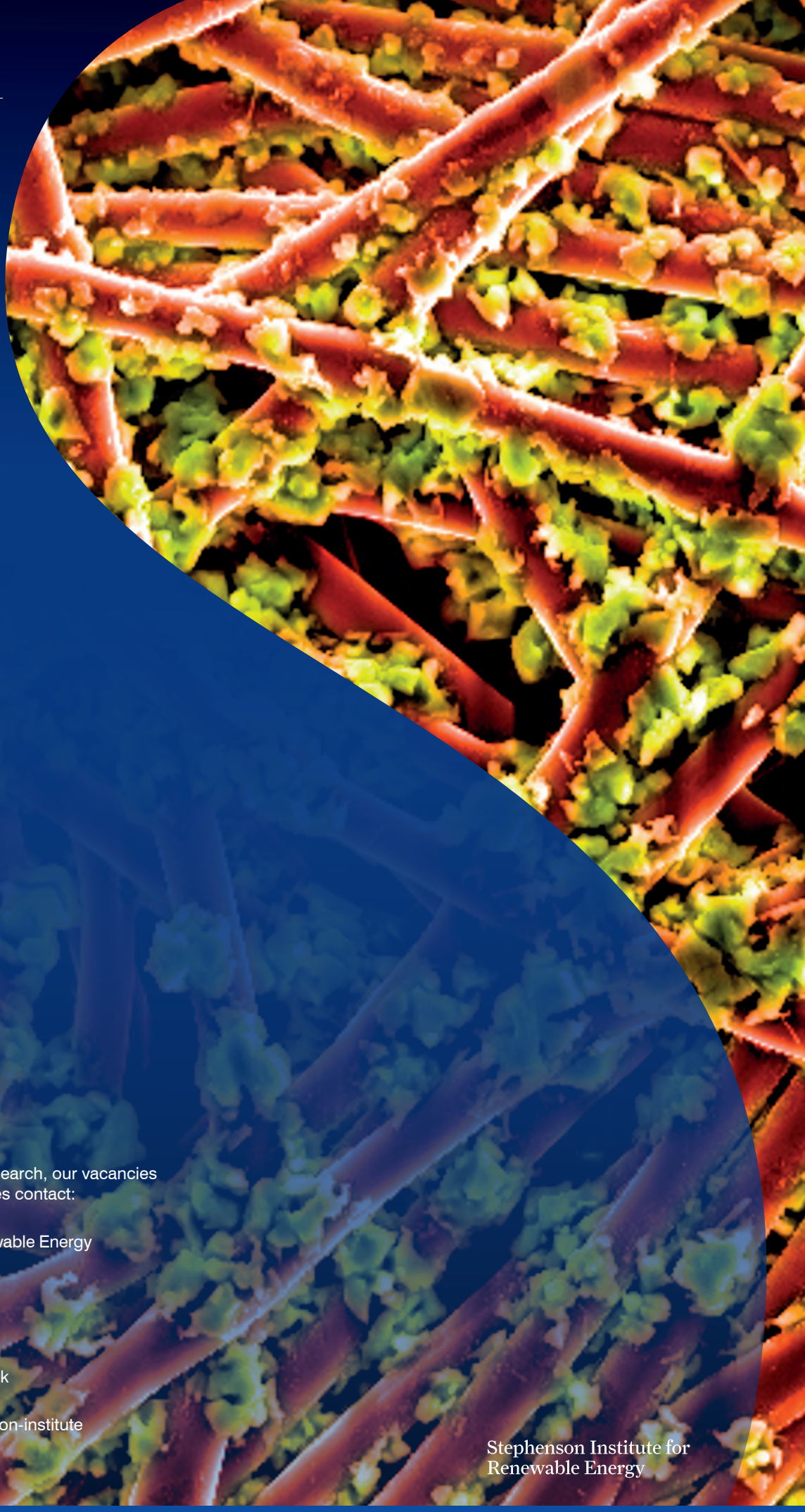
*L. J. Hardwick, A. J. Cowan and G. Teobaldi, Kerr gated Raman for the characterisation of SEI interface layers on battery electrodes,	**£40,000**

Staff Directory

Name	Email	Telephone	Subject
Alaria, Dr Jonathan	alariaj@liverpool.ac.uk	+44 (0)151 794 3366	Thermoelectrics and magnetism
Blanc, Dr Frédéric	frederic.blanc@liverpool.ac.uk	+44 (0)151 794 3511	NMR spectroscopy
Cowan, Dr Alexander	a.j.cowan@liverpool.ac.uk	+44 (0)151 794 3481	Electro- and photo-catalytic conversion
Dhanak, Prof Vin	vin@liverpool.ac.uk	+44 (0)151 795 0534/1	Photoemission of advanced materials
Durose, Prof Ken	ken.durose@liverpool.ac.uk	+44 (0)151 795 9048	PV materials and devices
Gründer, Dr Yvonne	Yvonne.Grunder@liverpool.ac.uk	+44 (0)151 795 2156	Fundamental electrochemistry
Hardwick, Prof Laurence	hardwick@liverpool.ac.uk	+44 (0)151 794 3493	Batteries and electrochemical interfaces
Hasell, Dr Tom	T.Hasell@liverpool.ac.uk	+44 (0)151 794 3502	Sulphur polymers for energy and sustainability
Jäckel, Dr Frank	fjaeckel@liverpool.ac.uk	+44 (0)151 795 2283	Nanocatalysis
Lopez-Sanchez, Prof Tony	jals@liverpool.ac.uk	+44 (0)151 794 3535	Bio-chemicals and catalytic conversion
Major, Dr Jon	jonmajor@liverpool.ac.uk	+44 (0) 151 795 9049	PV materials and devices
Sergeev, Dr Alexey	sergeev@liverpool.ac.uk	+44 (0)151 794 2665	Novel catalytic transformations
Shchukin, Prof Dmitry	d.shchukin@liverpool.ac.uk	+44 (0)151 795 2304	Nanoencapsulation
Veal, Prof Tim	t.veal@liverpool.ac.uk	+44 (0)151 794 3872	Semiconductor material physics

Back cover image: Elemental mapping using energy dispersive X-ray analysis of potassium superoxide grown on a carbon fibre electrode of a metal-oxygen battery (Dr Filipe Braga)

UNIVERSITY OF LIVERPOOL



Contact

To find out more about our research, our vacancies and postgraduate opportunities contact:

Stephenson Institute for Renewable Energy
The University of Liverpool
Chadwick Building
Peach Street
Liverpool L69 7ZF

T: +44 (0)151 79 5 8137
E: sire.support@liverpool.ac.uk

www.liverpool.ac.uk/stephenson-institute

Stephenson Institute for Renewable Energy

THE UNIVERSITY IS A MEMBER OF THE ELITE RUSSELL GROUP OF RESEARCH-LED UK UNIVERSITIES

WORLD LAND TRUST™