



UNIVERSITY OF  
LIVERPOOL

# Stephenson Institute

Annual Report 2019/20

Stephenson Institute for  
Renewable Energy

**LIFE CHANGING**  
World Shaping



# The Stephenson Institute for Renewable Energy

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The Annual Report 2019/20 was collated and edited by Jack Swallow, Leanne Jones, and Tim Veal

The article on page 5, featuring research by Professor Dmitry Shchukin, was first published in a longer format in the Horizon EU Research & Innovation magazine.

Front cover image: Optical microscopy of germanium selenide (Matthew Smiles)  
Contents page image: Optical microscopy of antimony selenide (Theo Hobson)  
Back cover image: Optical microscopy of antimony selenide (Nicole Fleck)



# Director's Welcome

Welcome to the SIRE Report for 2019/20 - a snapshot of our work on the chemistry and physics of energy storage, conversion, efficiency, and sustainability. Our objective is to work on topics that transform energy futures through fundamental science, understanding and controlling interfaces, new materials, and devices. With our unique focus on the physical sciences for energy research, we provide thought-leadership and research expertise on technologies such as solar energy, solar fuels, batteries and electrochemical capacitors. Our centre's research complements the large number of research groups and institutes that concentrate on engineering aspects of energy.

2019 was another outstanding year for SIRE. In particular, we welcomed two new academic members of SIRE: Dr Tom Hasell and Dr Andrea Vezzoli who have begun their lectureships in the Department of Chemistry and you can read about their exciting research areas within this report. SIRE increased its involvement with the newly established Faraday Institution through funding of two further projects on advanced battery characterisation and Li-ion positive electrode development. Our relationship with long-term industry partners Johnson Matthey, NSG and Unilever go from strength to strength with the award of jointly sponsored PhD studentships to begin in autumn 2020. Research from SIRE continues to have wider impact across society with the large-scale demonstration of thermo-regulating paint; to learn more turn to page 5.

Congratulations are in order for Professor Alex Cowan, promoted to a personal chair for his work in electro- and photo-catalytic conversion and solar fuels. Congratulations also to former members of SIRE who have recently secured lectureship positions and have embarked on their independent academic careers: Dr Iain Aldous at the University of Swansea, Dr Jyoti Gupta at Liverpool John Moores University, Dr Oliver Hutter at Northumbria University and Dr Tzu-Ho Wu at the National Yunlin University of Science and Technology, Taiwan.

It has been another busy period for PhD graduations. Eighteen of our early stage research colleagues successfully defended their theses in 2018 and 2019:

Nikolas Antonatos, Filipe Braga, Nick Brownbill, Jose Coco-Clemente, Josh Fogg, James Gibbon, David Herera, Martin Jacoobi, Liqaa Majdal, Silvia Mariotti, Stefano Mensa, Lena Reichenbach, Charlotte Smith, Jessica Stoner, Petar Radjenovic, Dong Xiao, Edgar Yañez, and Peter Yates. Their thesis titles and photos appear towards the end of this report. Every one in the team congratulates them and wishes them all well in their future careers!

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 researchers using the directory of expertise at the back of this report.

**Laurence Hardwick,**  
**SIRE Director**





# Impact and Events

## Next-Generation Batteries and Electrochemical Capacitors



Researchers at the Stephenson Institute for Renewable Energy (SIRE) are harnessing their battery expertise and knowledge to help answer the Industrial Strategy's Faraday Battery Challenge in five different projects, totalling over £5 million as part of this challenge, which aims to develop the next generation of batteries for vehicles and other applications.

Leading the SIRE charge are Professor Laurence Hardwick, the Institute's Director, and Professor Alex Cowan.

Professor Hardwick said: "The SIRE provides its expertise in battery material testing and advanced ex situ and operando characterisation. SIRE researchers are actively collaborating with other university and academic partners inside and outside of the UK, and taking advantage of state of the art facilities within the SIRE and the Materials Innovation Factory."

### UK battery research hubs

SIRE is a partner in four UK research hubs as part of the Faraday Battery Challenge, reflecting its position as one of the leading UK institutions for interdisciplinary energy storage research, in particular in the field of battery technologies.

### Li batteries for electric vehicles

Stephenson Institute for Renewable Energy is part of a new research consortium that has been awarded £11.2 million by the Faraday Institution to explore and develop new electrode materials for next-generation lithium batteries that can be used for electric vehicles.

The research aims to deliver improvements in the cost, performance and range of batteries used in electric vehicles, helping pave the way for zero emission transport.

### Safer batteries

A solid-state battery project is aiming to discover new solid state electrolytes for batteries, which in principle should be much safer than liquid electrolytes which are flammable. Professor Laurence Hardwick and Dr Fred Blanc will characterise the interfaces within these batteries using advanced optical spectroscopy and nuclear magnetic resonance. Other chemists Professor Matthew Rosseinsky, Dr John Claridge and Dr Matthew Dyer are working to discover new materials for this purpose.

The project will also test the feasibility of a solid state battery with performance superior to Lithium ion in electric vehicle applications. It will consider the barriers that are preventing the progression to market of solid-state batteries.

### Extending battery life

As part of the ISCF Faraday Battery Challenge grant, 'Extending battery life', the SIRE researchers are working in partnership with the STFC's Central Laser Facility. They are using Kerr-gated Raman spectroscopy to understand the battery degradation process in the hope of increased lifetime and better prediction of failure and working with over 10 UK partner Universities. The research is also making use of other national facilities, including the ISIS Neutron Source, the Diamond Light Source and, in collaboration with SIRE physicists, Professors Vin Dhanak and Tim Veal, the Research Complex at Harwell, in addition to SIRE photoemission facilities.

## Developing the Next Generation of Batteries and Electrochemical Capacitors

Awarded £5 Million in Faraday Battery Challenge



15 Universities + Companies Collaborating in 5 Major Projects



25+ Team of Researchers



Published 40+ Scientific Papers in Energy Storage



Advanced Battery Characterization: Over 10 Techniques



Advanced Battery Testing: Over 100+ Channels





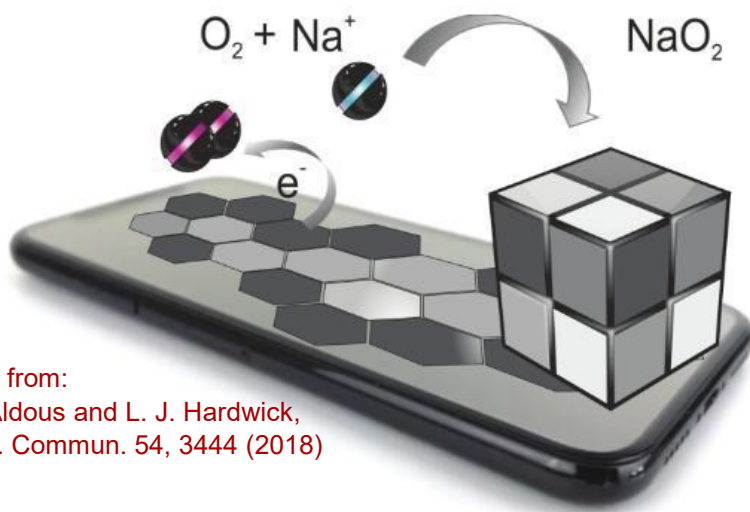


Image from:  
I. M. Aldous and L. J. Hardwick,  
*Chem. Commun.* 54, 3444 (2018)

### Identifying opportunities in Battery Characterisation

Laurence Hardwick and Nigel Browning Director of the Albert Crewe Microscopy Centre at Liverpool were commissioned by The Faraday Institution to undertake a scoping study. The recommendations from the report, entitled 'Identifying Infrastructure and Collaborative Expertise for Electrochemical Energy Storage Applications', are a foundation of the Faraday Battery Challenge, aiming to ignite a revolution in battery

research and accelerate the move to electric vehicles (EV).

Professor Nigel Browning (Schools of Engineering and Physical Sciences) said: "By coordinating researchers together in the characterisation of energy storage systems, the Faraday Institution has a tremendous opportunity to establish unique expertise in the UK and accelerate the insights needed to innovate world-leading devices."

The scoping study has led to a

### SuperCap Impact in Electrochemical Capacitors

SIRE is part of a £2.2M consortium funded by ISCF Faraday Battery Challenge Innovation grant "G-Cap supercapacitor in all-terrain vehicle" with industrial partners RDGraphene, MEP Technologies and Agile Vehicle Technologies, where we will develop the next generation of EV batteries that are augmented by graphene supercapacitors ("G-Cap") to yield high-power and high-energy systems.

## European Research Council Project Impact: Paint that heats homes

Applying a coat of paint on the walls of a house may soon help to heat it, saving energy and reducing  $CO_2$  emissions.

In Europe, half of cities' annual energy consumption goes to heating and cooling. Despite the EU's move towards decarbonisation, 75% of heating and cooling comes from fossil fuels, whilst only 19% is generated from renewable energy.

Prof Dmitry Shchukin's group from the Stephenson Institute for Renewable Energy have developed a thermo-regulating paint that can absorb and release heat inside brick buildings, keeping rooms warm whenever necessary by using excess energy. The paint, which was developed as part of a project called ENERPAIN, could be used as a form of insulation to increase the energy efficiency of old houses at low cost.



### Phase-change materials

Prof Shchukin said 'Paint and coating manufacturers have their own paints and we just supply some additives, about 5%, to the paint.'

These additives are so-called phase-change materials (PCMs), such as paraffins, salt hydrates and fatty acids, encased in protective nanometre-sized capsules which improve heat transfer. PCMs can store large amounts of thermal energy and change states, from solid to liquid and vice versa, without altering their own temperature.

Developing this paint, which is currently being tested, is part of a wider project called ENERCAPSULE, where Professor Shchukin is designing suitable coatings to encapsulate PCMs at the nanoscale to use in paints, textiles and medicines. 'For the paints, we used salt hydrates due to their low cost and very high volumetric energy storage density,' said Professor Shchukin. 'However, these were very difficult to encapsulate as they are corrosive and hydrophilic.' He was able to enclose salt hydrates in polymer shells as small as 10 nm, which protects them from the surrounding environment but also allows them to respond to the heat in a controlled way. He says European, Chinese and Russian companies are showing interest in their research, and that he now hopes to make nanocapsules for paints that can help cool buildings.



# EPSRC Centre for Doctoral Training in New and Sustainable Photovoltaics – CDT-PV

## EPSRC

Pioneering research  
and skills



CENTRE FOR DOCTORAL TRAINING  
NEW AND SUSTAINABLE  
PHOTOVOLTAICS

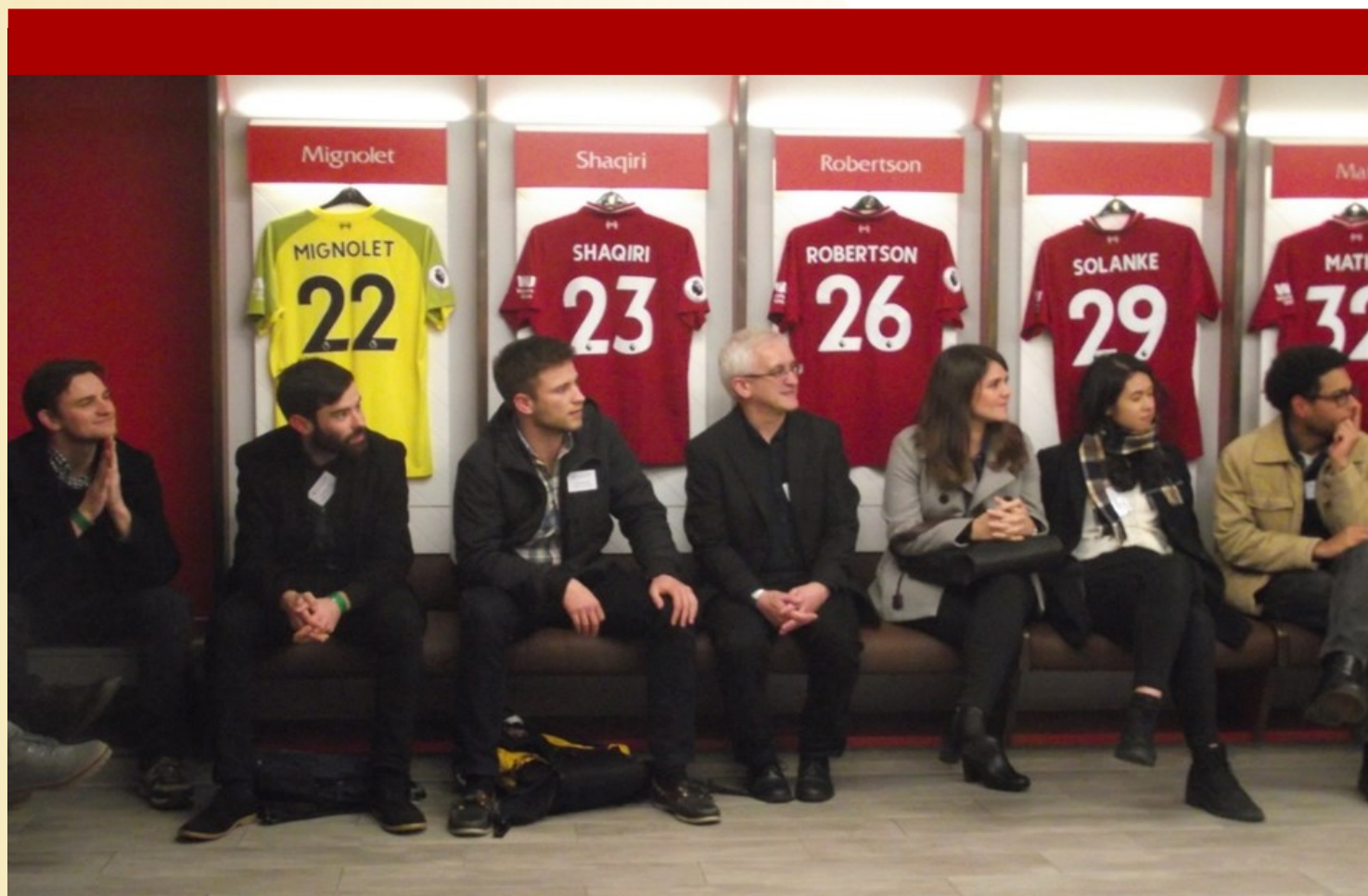
The Centre for Doctoral Training in New and Sustainable Photovoltaics (CDT-PV) is a UK national centre having the mission of training future leaders for research and industry in solar energy generation. Our central theme is that the next generation of solar photovoltaic panels will be able to satisfy the needs of both the mass market and for specialist products. These solar cells will need to be made from the new and sustainable materials that are the focus of our research and training. The CDT-PV is led from Liverpool and comprises seven partner universities, giving complete coverage of the research themes and training

needs relevant to the future of solar electricity generation.

### CDT-PV Showcase

A regular feature of the Centre's activities is its annual showcase, where the students not only get the opportunity to present their work but also become involved in the organisation of the symposium. In November 2018 the CDT-PV Showcase was held at Anfield Stadium in Liverpool, and was attended by 90 students, academics and industrial panel members, including Dr Phil Dale from the University of Luxembourg, who is one of our International Advisors. The event was organised in conjunction with

the students from the fourth cohort and the chair was Leo Buizza, a student at University of Oxford. There was a great line up of invited speakers, including Dr Sian Dutton, University of Cambridge who gave a talk on structural (dis)order as a pathway to functional materials for lithium ion cells and Prof Trystan Watson from Swansea University spoke about the challenges of manufacturing scale up for perovskite solar cells. Dr Robert Hoyer from University of Cambridge presented his work on bismuth-based solar cell materials. Arfa Karani spoke about her work on perovskite solar cells and solar power in the developing world.



Caption: During the tour of Anfield, CDT-PV Showcase 2018

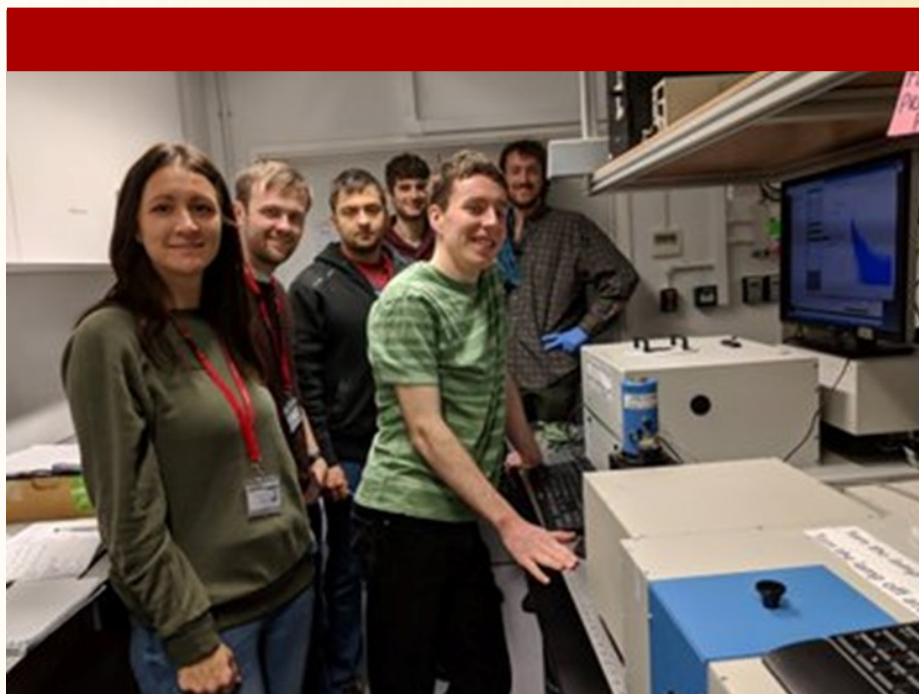


All CDT-PV students gave research presentations, with seven students giving talks and the remainder presenting posters. Our tradition is to award prizes with the jury comprising the most recent cohort of students to join the Centre. The winning presentation was by Alan Bowman (Cambridge) on Spectroscopic Studies of Low-Bandgap Perovskite films. The runner-up was Leo Buizza (Oxford), who also won the poster prize. The day was pleasantly concluded by a tour of the stadium followed by the conference dinner.

### Training events in 2019

The 2019 intake was a particularly large cohort of 17 PhD students (including two affiliates). Our core training programme started with an intensive course at Liverpool before the students paid two-week visits to each of the partner labs of Bath, Cambridge, Loughborough, Oxford, Sheffield, and Southampton. As always, this was a real highlight for the students, where they have the opportunity to gain a wide range of knowledge and skills relating to photovoltaics from leading academics from each of the partners.

The CDT-PV has continued to be active in organising annual training events in conjunction with the SUPERGEN Solar hub to train students and post-docs in essential specialist knowledge/techniques relating to photovoltaics. This year the event was held at the University of Warwick on the topic of PV materials and characterisation. Almost 40 attendees listened to 7 presentations from leading academics on topics such as inorganic materials, transparent conducting oxides, optical spectroscopy and electron microscopy. This also provided a forum for CDT-PV students and academics to connect with researchers from other universities and from industry. Also this year, the CDT-PV supported a one day Perovskite symposium held at the



Cohort 5 in the Labs during the University of Oxford training module

University of Oxford, where a number of our students participated and presented posters.

### CDT-PV Summer School & Showcase 2019

In September 2019, the CDT-PV Summer School and Showcase event were both held at the University of Bath with the most recent cohort of students to join the CDT having a big hand in its organisation with the local academic leader at Bath, Prof Alison Walker, the CDT's Academic Director. A total of 65 people attended the events across the week, including external guests. The three-day Summer School included talks about thesis writing and viva preparations delivered by Prof Ken Durose and supported by Prof Alison Walker. Dr Finlay Colville delivered an excellent presentation about industry trends in the photovoltaics market. Other invited speakers included Dr KT Tan (Viridian Solar), Dr Stuart Boden (black silicon, Univ. Southampton), Prof Matt Rosseinsky (materials discovery, Univ. Liverpool) and Kate Levick (renewable energy and climate politics, E3G). Prof Laurie Peter (Bath) gave an overview talk about solar fuels. Dr Joe Walsh and Dr Jenny Cooper spoke about their experiences in industry, working for large companies based in the UK.

A further highlight of the week was the Researcher Forum organised by Kaya Brechley (Bath) and Matthew Smiles (Liverpool) which featured break-out groups focussing on key topics in solar research. They also organised a lively panel discussion on careers and workplace experiences with Dr Annette Pressman (Thomson Reuters), Dr Jon Major (Univ. Liverpool), Dr Oliver Weber (Oxford PV) and Dr Andy Chalmers (Univ. Bath & CiteAb). Evening activities included group meals in Bath and a CDT-PV quiz.

This Showcase was led by Dan Sowood (Cambridge) and his colleagues from the CDT's fifth cohort. The student presentations were of an exceptional standard, on a par with that at any high calibre international conference. The event ended with prize giving, with Joel Smith (Sheffield) winning the Best Presentation award and Tom Featherstone (Liverpool) the runner up. Best poster award went to Francesco Bastiani (Sheffield), with Luke Thomas (Liverpool) the runner up.



# SIRE Seminar Series 2018/2019

All staff in the SIRE would like to thank the seminar speakers for 2018/2019.

Our seminars are open to all. Details of the current programme can be found at

[www.liverpool.ac.uk/renewable-energy/events/](http://www.liverpool.ac.uk/renewable-energy/events/)

| Date                           | Speaker                  | Institution                                               | Title                                                                                                                                                |
|--------------------------------|--------------------------|-----------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------|
| 17 <sup>th</sup> July 2019     | Mr Max Mann              | Flinders University, Adelaide, Australia                  | Low-Cost Polysulfide Polymers as Sorbents for Mercury-Free Subsistence and Small Scale Gold Mining and Controlled-Release Fertilisers                |
| 16 <sup>th</sup> July 2019     | Prof Ellen Backus        | University of Vienna, Austria                             | Ultrafast SFG Study towards Water Splitting on TiO <sub>2</sub>                                                                                      |
| 3 <sup>rd</sup> July 2019      | Dr Goutam Kumar Dalapati | SRM University-AP, India                                  | Nanostructure incorporated photovoltaics for renewable energy application: CuO, CZTS and metallic transparent conductors                             |
| 2 <sup>nd</sup> April 2019     | Dr Leigh Aldous          | King's College, London                                    | Using redox chemistry and entropy for waste heat harvesting via the thermogalvanic effect                                                            |
| 26 <sup>th</sup> March 2019    | Dr Johan Jacquemin       | Queens University Belfast                                 | In-Silico Evaluation of the Transport Properties of Electrolytes for Energy Storage Applications                                                     |
| 12 <sup>th</sup> March 2019    | Dr Lee Johnson           | University of Nottingham                                  | The Rechargeable Aprotic Li-O <sub>2</sub> Battery                                                                                                   |
| 19 <sup>th</sup> February 2019 | Prof. Jian-Feng Li       | Xiamen University, China                                  | Probing Surface Reaction and Intermediates using In Situ Raman Spectroscopy                                                                          |
| 12 <sup>th</sup> February 2019 | Dr Karen Johnston        | University of Durham                                      | Probing Ion Mobility Mechanisms in Solid Electrolytes using Solid-State NMR Spectroscopy                                                             |
| 5 <sup>th</sup> February 2019  | Dr Stijn Mertens         | Lancaster University                                      | From Collective to Single-Molecule Switching in 2D Materials at Solid-Liquid Interfaces                                                              |
| 29 <sup>th</sup> January 2019  | Dr Ainara Aguiadero      | Imperial College, London                                  | Local chemical degradation processes and ionic transport in garnet all-solid-state batteries                                                         |
| 4 <sup>th</sup> December 2018  | Prof Peter Weightman     | University of Liverpool                                   | Funding for research on the FELIX free electron lasers                                                                                               |
| 3 <sup>rd</sup> December 2018  | Nian Lin                 | Hong Kong University of Science and Technology, Hong Kong | Metal-organic coordination on surfaces: towards complexity and functionality                                                                         |
| 20 <sup>th</sup> November 2018 | Dr Paul Donaldson        | STFC-UKRI Rutherford Appleton Laboratory                  | Adventures in ultrafast laser spectroscopy at the CLF. New multidimensional IR techniques and new applications in heterogeneous catalysis            |
| 13 <sup>th</sup> November 2018 | Jessica Stoner           | University of Liverpool                                   | Chemical Control of Correlated Metals as Transparent Conductors                                                                                      |
| 16 <sup>th</sup> October 2018  | Dr Peter Priece          | University of Liverpool                                   | Microwave-assisted heterogeneous catalysis in biomass conversion                                                                                     |
| 9 <sup>th</sup> October 2018   | Dr Brant Walkley         | University of Sheffield                                   | Materials for a sustainable future: Composition-'local-structure'-property relationships in materials for energy production, storage and remediation |



# Research Group Expertise and Highlights

## Cystal Growth, Magnetism and Thermoelectrics

Jonathan Alaria

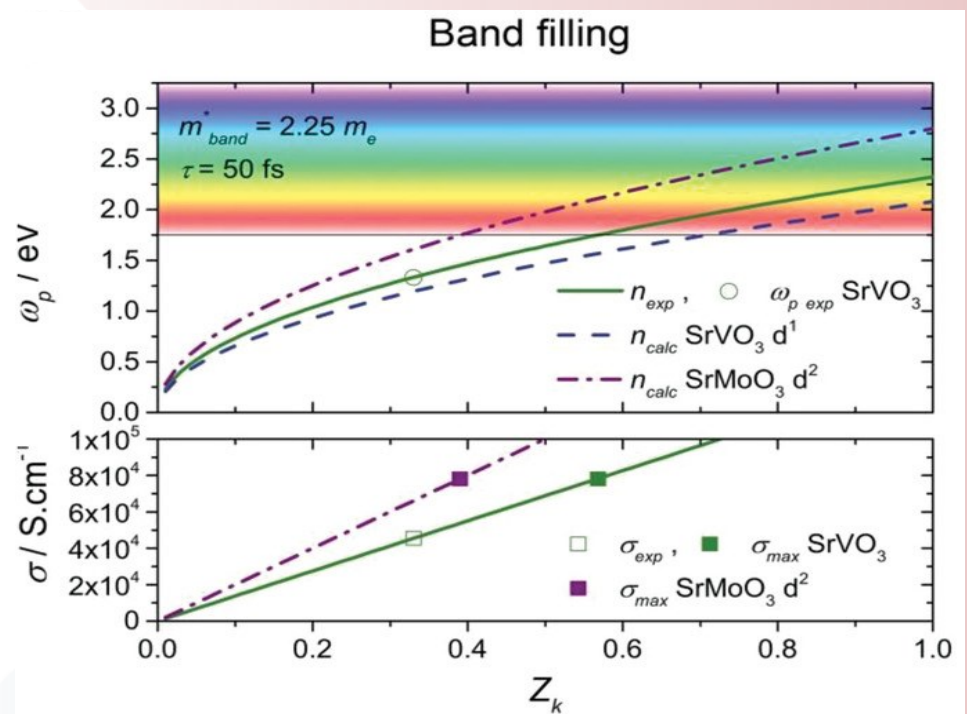
We specialise in single crystal bulk growth, thin film growth by pulsed laser deposition and physical characterisation. High quality crystals are an essential part of our research, enabling us to determine fundamental properties of new or previously misunderstood materials. Physics understanding and 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: Chemical Control of Correlated Metals as Transparent Conductors

Correlated metallic transition metal oxides offer a route to thin film transparent conductors that is distinct from the degenerate doping of broadband wide gap semiconductors. In a correlated metal transparent conductor, interelectron repulsion shifts the plasma frequency out of the visible region to enhance optical transmission, while the high carrier density of a metal retains sufficient conductivity. By exploiting control of the filling, position, and width of the bands derived from the B site transition metal in  $ABO_3$  perovskite oxide films, it is shown that pulsed laser deposition-grown films of cubic  $SrMoO_3$  and orthorhombic  $CaMoO_3$  based on the second transition series cation  $4d^2 Mo^{4+}$  have superior

transparent conductor properties to those of the first transition series  $3d^1 V^{4+}$ -based  $SrVO_3$ . The increased carrier concentration offered by the greater band filling in the molybdates gives higher conductivity while retaining sufficient correlation to keep the plasma edge below the visible region. The reduced binding energy of the  $n=4$  frontier orbitals in the second transition series materials shifts the energies of oxide  $2p$  to metal  $nd$  transitions into the near-ultraviolet to

enhance visible transparency. The A site size-driven rotation of  $MoO_6$  octahedra in  $CaMoO_3$  optimizes the balance between plasma frequency and conductivity for transparent conductor performance.



Plasma frequency  $\omega_p$  as a function of the renormalization factor  $Z_k$  for the theoretical (blue line) and reported (green line) carrier concentration of  $3d^1$   $SrVO_3$  and for the theoretical carrier concentration of  $4d^2$   $SrMoO_3$  (purple line). The experimental plasma frequency reported for  $SrVO_3$  with  $Z_k = 0.33$  is represented with an open green circle. Bottom panel: Conductivity  $\sigma$  as a function of  $Z_k$  with a scattering factor  $\tau = 50$  fs, to account for the measured mobility, and the reported carrier concentration of  $SrVO_3$  (green line) and for the theoretical carrier concentration of the  $4d^2$   $SrMoO_3$  (purple line). Published under a Creative Commons Attribution License in *Advanced Functional Materials* **29**, 1808609 (2019)



# Magnetic Resonance in Solids for Energy Materials and Catalysis

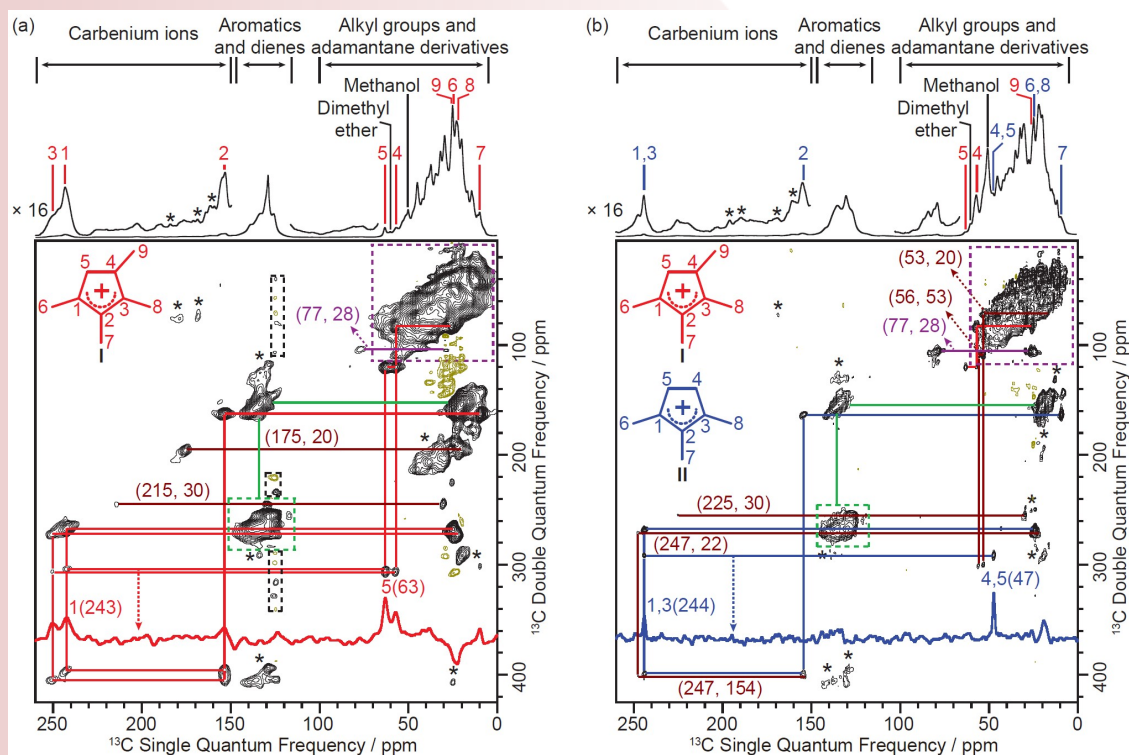
Frédéric Blanc

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.

## Highlight: Identification of Different Carbenium Ion Intermediates in Zeolites with Identical Chabazite Topology via $^{13}\text{C}$ - $^{13}\text{C}$ Through-Bond NMR Correlations

The production of light olefins via the methanol-to-olefins (MTO) reaction is an important chemical process that links non-oil resources such as coal and natural gas with olefin-based petrochemicals. This reaction is catalysed microporous acidic zeolites amongst which H-SAPO-34, a silicoaluminophosphate zeolite with the chabazite (CHA) topology, is of particular importance due to its high selectivity to ethylene and propene, and is of commercial use. H-SSZ-13 is also a CHA silicoaluminate analogue of H-

SAPO-34 which has been shown to be a potential alternative in the MTO process. In collaboration with colleagues at Dalian Institute of Chemical Physics (DICP) in China and using advanced NMR techniques providing  $^{13}\text{C}$  –  $^{13}\text{C}$  through bond correlation, we have captured in the act the carbenium ion intermediates stabilised in the two different zeolites during the MTO reaction and revealed that these are different despite that the zeolites possess identical CHA. The cations identified offer a more comprehensive understanding of the reaction routes and will inspire future researches on their roles in MTO processes.



2D  $^{13}\text{C}$ – $^{13}\text{C}$  refocused INADEQUATE spectra of activated (a) H-SSZ-13 and (b) H-SAPO-34. The assignments of the different carbenium ions and their corresponding structures are coloured-coded. Some representative traces extracted along the horizontal dimension are also shown. The correlations coded in green and purple belong to the neutral species (aromatics, dienes and adamantane derivatives). Numbers in parenthesis are the chemical shifts of the correlated  $^{13}\text{C}$  sites. Asterisks (\*) denote spinning sidebands.

Xiao et al., RSC Advances **9**, 12415-12418 (2019) – Published by the Royal Society of Chemistry under a Creative Commons Attribution 3.0 Licence.

# 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<sub>2</sub> 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 the mecha-

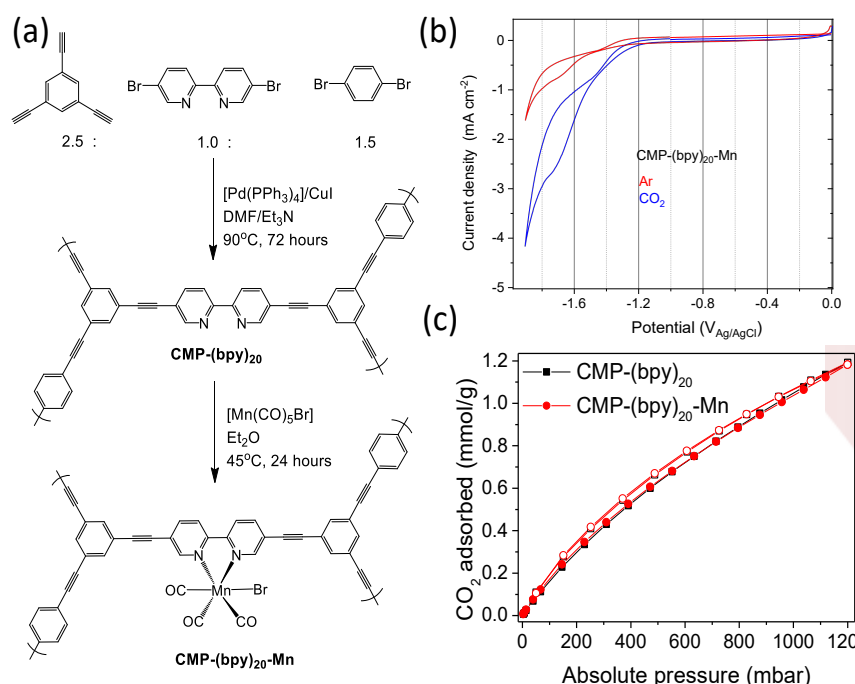
nisms of renewable energy materials. We have expertise in transient absorption spectroscopy, a technique that enables the study of light induced processes to study charge carrier dynamics in solar energy conversion materials. We also utilise vibrational sum-frequency generation (SFG) spectroscopy to study the surface mechanisms at electrodes for (photo)electrocatalysis and energy storage.

## Highlight: Porous materials for integrated CO<sub>2</sub> capture and Conversion

The capture and electrochemical conversion of carbon dioxide (CO<sub>2</sub>)

offers an exciting chance to generate low-carbon fuels. Typically capture is carried out, the CO<sub>2</sub> purified and compressed, then transported prior to conversion with individual steps being costly and in some cases energy intensive. Here we demonstrated how a CO<sub>2</sub> reduction electrocatalyst based on a low cost manganese metal centre can be covalently bound in a conjugated microporous polymer (CMP). CMP's were first developed at Liverpool in the Chemistry department by one of the investigator team (Prof Cooper) and are an emerging CO<sub>2</sub> capture material. For the first time we were able to show that the hybrid catalyst-CMP could act as both a CO<sub>2</sub> uptake material and an electroactive support for the Mn catalytic centres, providing a pathway towards integrated materials for the capture and conversion of dilute CO<sub>2</sub> sources.

Synthetic pathway to produce the high surface area (549 m<sup>2</sup> g<sup>-1</sup>) conjugated microporous polymer containing the Mn catalytic centre (a). Enhanced currents are observed under CO<sub>2</sub> indicating the catalyst centre remains electroactive (b) and the CO<sub>2</sub> adsorption-desorption isotherms measured show no loss in gas uptake upon addition of the catalyst centre. Figure Adapted from Sustainable Energy Fuels 3, 2990-2994, (2019) with permission from The Royal Society of Chemistry.



## Photoemission Characterisation of Energy Materials

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, as well as the density of states on either side of the Fermi level. We

also synthesis copper zinc tin sulphide and related PV absorbers by chemical bath, spray pyrolysis and magnetron sputter techniques. In addition, the ultrahigh vacuum systems in our laboratory also have scanning tunnelling microscopy and low energy electron diffraction capabilities for surface structural studies.

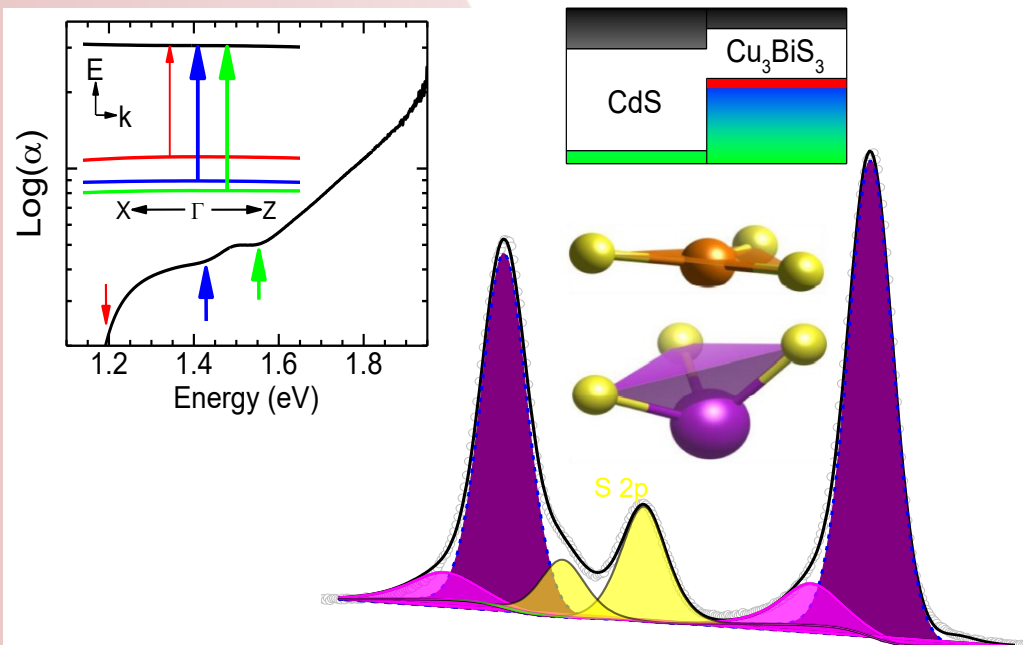


## Highlight: $\text{Cu}_3\text{BiS}_3$ Properties for Photovoltaics

The earth-abundant semiconductor  $\text{Cu}_3\text{BiS}_3$  (CBS) exhibits promising photovoltaic properties and is often considered analogous to the solar absorbers copper indium gallium diselenide (CIGS) and copper zinc tin sulfide (CZTS) despite few device reports. The extent to which this is justifiable is explored via a thorough x-ray photoemission spectroscopy (XPS) analysis: spanning core levels,

ionization potential, work function, surface contamination, cleaning, band alignment, and valence-band density of states. The XPS analysis overcomes and addresses the shortcomings of prior XPS studies of this material. Density functional theory (DFT) calculations of the band structure inform the interpretation of optical transmission and Raman spectra. Valence band XPS spectra and DFT calculations find the CBS bonding to be superficially similar to CIGS and CZTS, but the  $\text{Bi}^{3+}$  cations have fun-

damental impacts: giving a low ionization potential (4.98 eV), suggesting that the CdS window layer favoured for CIGS and CZTS gives detrimental band alignment and should be rejected in favor of a better aligned material in order for CBS devices to progress. The study shows that using a greater knowledge of the underlying electronic structure in materials like CBS can help in a redesign of solar cell architecture.



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XPS spectra for the Bi 4f and S 2p overlap region of the  $\text{Cu}_3\text{BiS}_3$  (CBS) sample after surface cleaning. Peak envelope is shown in black; Optical absorption spectra from CBS and a schematic representation of the band structure and absorption transitions at the  $\Gamma$  point; Vacuum-aligned band diagram between CBS and the common n-type partner material, CdS.

## Solar energy materials and solar cells

### Ken Durose

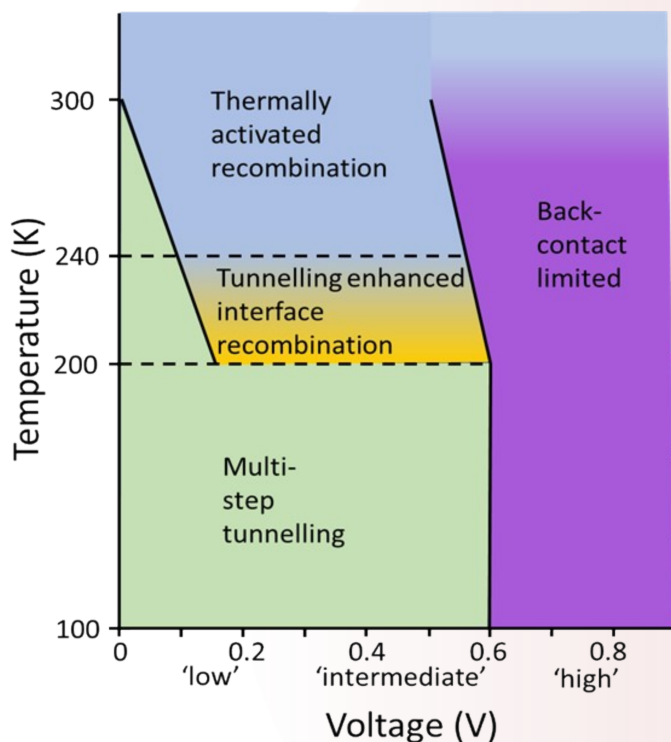
The group focusses on low cost thin film photovoltaic materials and devices for solar electricity generation. In particular we investigate new and emerging materials that could have the potential to compete with silicon solar modules as a major source of energy. Our experimental activities span the complete range of thin film deposition methods required to make solar cells and also includes the characterisation needed to understand both the fundamental behaviour of the materials and the performance of solar cell devices. The key part of any solar cell is the light-absorbing layer. While our group is well-known for its work on CdTe, we have also run projects on  $\text{Sb}_2\text{Se}_3$ ,  $\text{CuSbS}_2$ , all-inorganic perov-

skites including  $\text{CsPbI}_2\text{Br}$  and  $\text{Cs}_2\text{TeI}_6$  and organic partner layers for use in heterostructures or as electrical contacts. We have an unusually wide materials capability that gives us considerable flexibility in the design of new photovoltaic structures. The group collaborates extensively within SIRE where there are productive overlaps in expertise and cross-working on joint projects.

### Highlight: Current transport analysis in CdTe solar cells

Solar cells operate by allowing photogenerated charge carriers from sunlight to be swept aside by the built-in field of a semiconductor  $p$ - $n$  diode. In the ideal case the current-

voltage response of the diode is described by the 'diode equation', and this curve describes the maximal performance of a solar cell. However, in practice a range of physical effects can limit the movement of charge through the solar cell, and hence reduce its performance. Our collaborators Habibe and Murat Bayhan, from Mugla University, Turkey are regular visitors to our laboratory and are experts in current transport analysis of solar cells. In this work they measured the temperature dependence of the current-voltage of CdTe devices and compared their mathematical forms to those expected for different physical current transport mechanisms.



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Regimes of current transport in a CdTe solar cell plotted on a Temperature – Voltage field

The results are shown in the figure above which presents a map of the temperature and voltage regimes in which different transport mechanisms operate. Since solar cells usually operate at  $T > 300$  K and at voltages  $> 0.5$  V, it can be seen from the

figure that the low temperature tunnelling mechanisms are not of practical importance. Instead the solar cells are likely to run in the more nearly-ideal 'thermally activated' regime but there are potentially problems with non-Ohmic contacts.

The work has taken this approach as far as it can go with this kind of solar cell device in highlighting the regimes of current transport that operate in practical devices.

## 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 a new experimental set-up allow us to characterise electrochemical interfaces *in situ*, including their potential-

and time-dependence, in order to link structure, reactivity and stability.

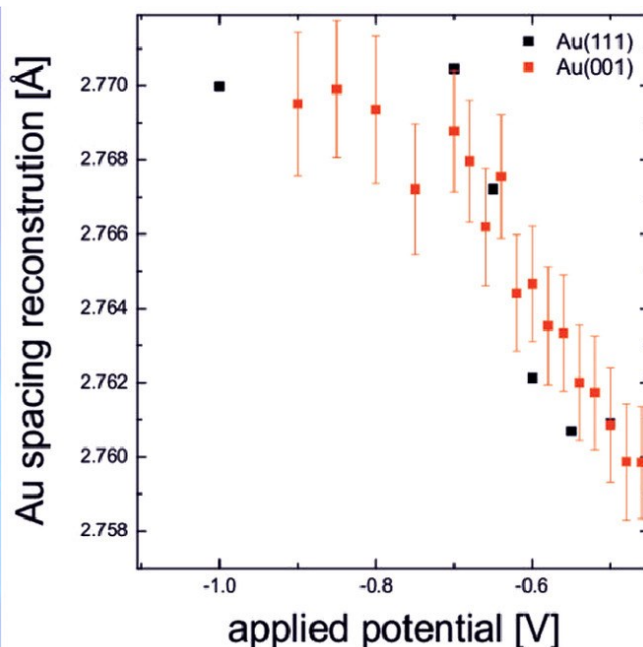
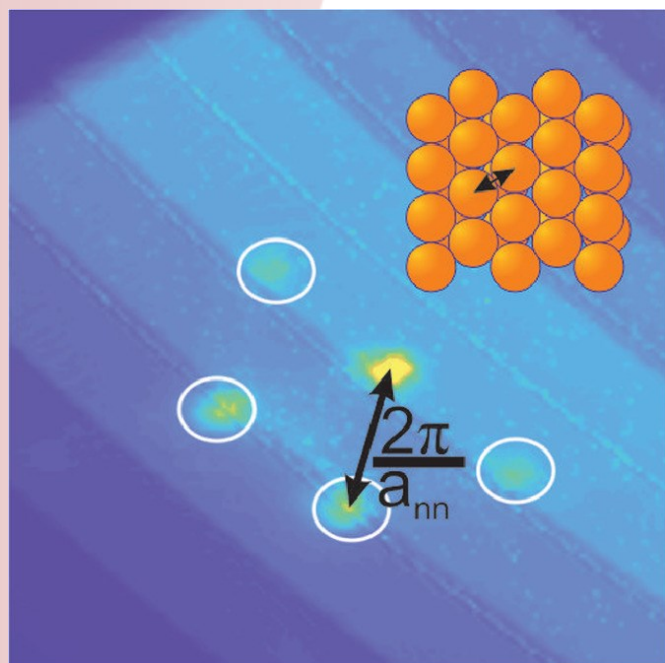
### Highlight: Potential-dependent Surface Compression of Gold and its Link to Electrocatalytic Reactivity

The surfaces of gold exhibit a rich physical behaviour that is interesting, not only from a structural perspective, but also for applications in areas such as heterogeneous catalysis and electrocatalysis. In this paper, we show that the hexagonal reconstructions of both the Au(111) and the cubic Au (001) surfaces in alkaline electrolyte exhibit a potential-dependent in-plane compression that is remarkably similar despite the substantial difference in the geometry of the underlying substrate.

The compressibility is linked to the charge on the surface Au atoms within a simple free electron model. The interplay between surface charge and the adsorption of hydroxide species determines both the surface compression and the reversible lifting of the reconstructions. In the presence of adsorbed carbon monoxide, both the potential-induced changes in the surface compression and the lifting of the reconstruction are suppressed, leading to the promotion of electrocatalytic reactivity.

Y. Gründer, G. S. Harlow, E. Cocklin, J. Fogg, J. W. Beane, and C. A. Lucas, *Surface Science* **680**, 113-118 (2019)





A schematic of the gold reconstruction on the Au(111) electrode in real and reciprocal space is shown. The change in the peak position is a direct measurement of the gold atom spacing in the reconstructed surface as function of the applied electrochemical potential. Reproduced with permission under license number: 4684180342929 from Y. Gründer, G. S. Harlow, E. Cocklin, J. Fogg, J. W. Beane, and C. A. Lucas, *Surface Science* **680**, 113-118 (2019)

## Advanced In situ and Operando Characterisation of Battery Materials

Laurence Hardwick

Lithium ion batteries have revolutionised technological progress of the past two decades. Developing both new types of batteries (with higher energy storage and superior performance) and optimising existing Li-ion technology for longer life is crucial for the realization of a true alternative to a fossil-fuel-based energy economy.

**Highlight: Kerr-gated Raman spectroscopy of LiPF<sub>6</sub> salt and LiPF<sub>6</sub>-based organic carbonate electrolyte for Li-ion batteries**

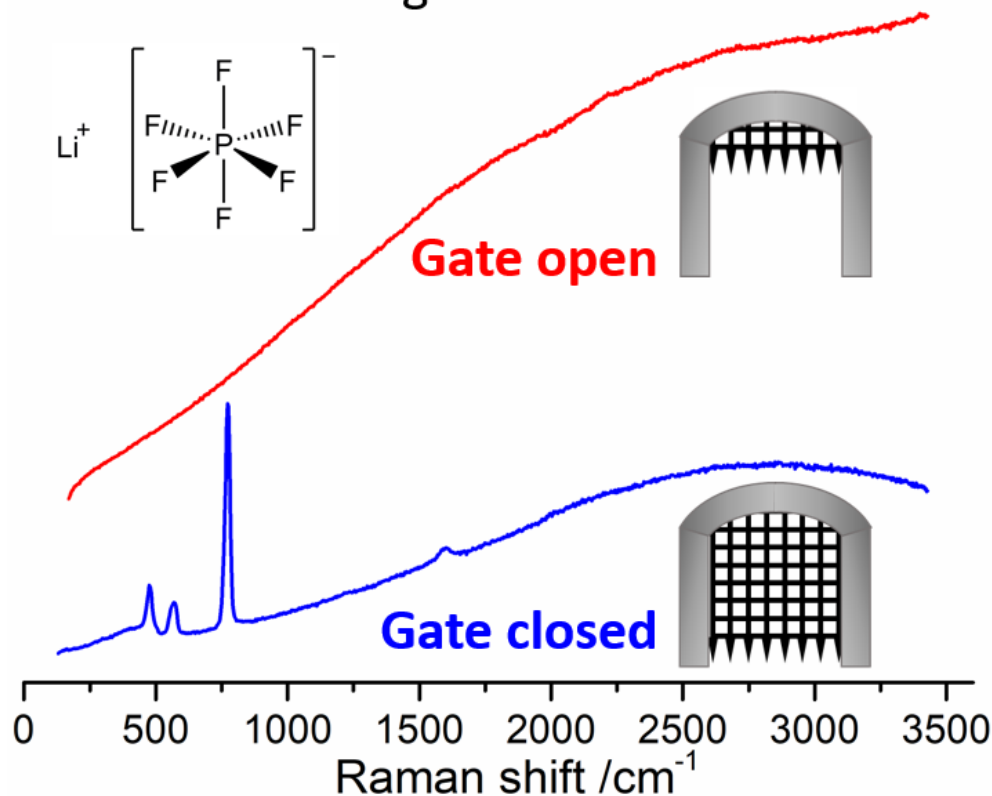
Fluorescent species are formed during cycling of lithium ion batteries as a result of electrolyte decomposition due to the instability of the

non-aqueous electrolytes and side reactions that occur at the electrode surface. The increase in the background fluorescence due to the presence of these components makes it harder to analyse data due to the spectroscopic overlap of Raman scattering and fluorescence. Herein, we demonstrate that Kerr-gated Raman spectroscopy to be an effective technique for the isolation of the scattering effect from the fluorescence enabling the collection of the Raman spectra of LiPF<sub>6</sub> salt and LiPF<sub>6</sub>-based organic carbonate electrolyte, without the interference of the fluorescence component. Kerr gated Raman was able to identify POF<sub>3</sub> on the LiPF<sub>6</sub> particle surface, after the addition of trace water.

Our study highlights Kerr-gated Raman as a powerful technique that can be applied in the investigation of electrode/electrolyte interfaces and the speciation of the solid electrolyte interphase of battery systems in ex situ or operando studies, even in the presence of fluorescent species formed during cycling due to the suppression of the background emission.

L. Cabo-Fernandez, A. R. Neale, F. Braga, I. V. Sazanovich, R. Kostecki and L. J. Hardwick *Phys. Chem. Chem. Phys.* **21** (2019) 23833-23842.

## Kerr gated Raman



Partial and complete suppression of the fluorescence signals originating from degradation products and impurities in Li-ion electrolyte materials was achieved with the Kerr gate, revealing the Raman signals and chemical information hidden beneath.

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## Functional Porous Materials from Inorganic Waste

Tom Hasell

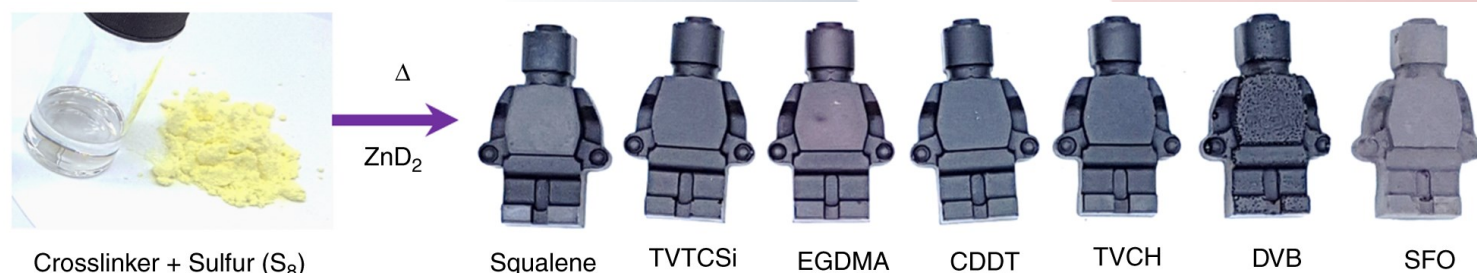
Porous materials are permeable, high surface area materials with applications in gas storage, catalysis, and filtration. There has been considerable interest in porous materials over the last ten years, and metal-organic frameworks and porous polymers with incredible properties have been reported. However, many of these new materials are limited in application due to the high cost of production. We are developing new porous materials from inorganic waste and other low cost or renewable resources. The target is to produce materials with superior properties, but at a cost that makes them useful for widespread practical applications, espe-

cially filtration of toxic pollutants from water and air flows. A good example is sulphur-polymers. Sulfur is an industrial by-product of oil refining. We recently showed that when polymers made from elemental sulfur are made porous, they can be used to filter mercury from water.

### Catalytic inverse vulcanization

The discovery of inverse vulcanization has allowed stable polymers to be made from elemental sulfur, an unwanted by-product of the petrochemicals industry. However, further development of both the chemistry and applications is handicapped by the restricted choice of cross-linkers

and the elevated temperatures required for polymerisation. Here we report the catalysis of inverse vulcanization reactions. This catalytic method is effective for a wide range of crosslinkers, reduces the required reaction temperature and reaction time, prevents harmful  $\text{H}_2\text{S}$  production, increases yield, improves properties, and allows otherwise unreactive crosslinkers to be used. Thus, inverse vulcanization becomes more widely applicable, efficient, eco-friendly and productive than the previous routes, not only broadening the fundamental chemistry itself, but also opening the door for the industrialization and broad application of these fascinating materials.



A crosslinker (EGDMA) and elemental sulfur and examples of molded objects of catalyzed thiopolymers.

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# 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 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

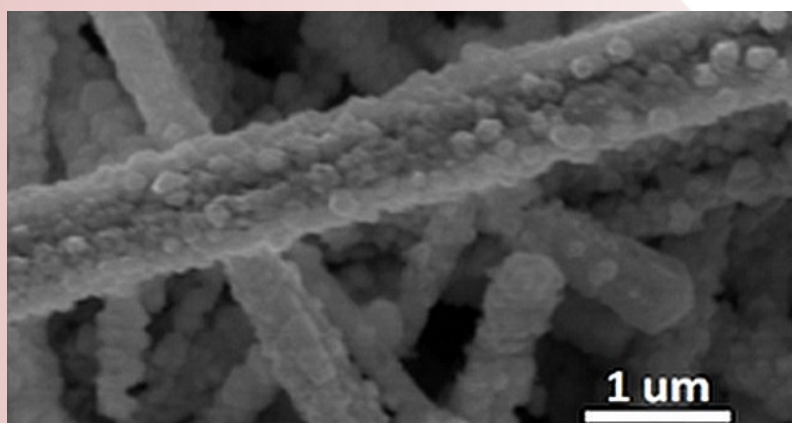
nanophotonics.

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.

## Highlight: Cu/Cu<sub>2</sub>O Core-Shell Nanowires for solar hydrogen

Solar hydrogen is considered as component in a future sustainable energy mix. In this research, we

developed a fast and straight forward wet chemical synthesis route to Cu/Cu<sub>2</sub>O core-shell nanowires suitable as a photocathode material for photoelectrochemical water splitting. Using an ultrathin (11 nm) protective coating and a earth-abundant non-toxic nickel based co-catalyst we achieved hydrogen generation efficiencies comparable to other CuO<sub>2</sub>-based photocathodes employing noble metal co-catalysts and thicker protective coatings. This is an important step towards large scale application of this material in solar hydrogen generation.



Scanning electron micrograph of Cu/Cu<sub>2</sub>O core shell nanowires decorated with a nickel-based co-catalyst for solar hydrogen generation.

Chemically Synthesized Cu/Cu<sub>2</sub>O Core-Shell Nanowire-Based Photocathode for Efficient and Durable Photoelectrochemical Hydrogen Generation (2019)

# 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<sub>2</sub>. 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: Economic and agronomic impact assessment of wheat straw based alkyl polyglucoside produced using green chemical approaches

We quantified the economic feasibility and resource efficiency charac-

teristics of producing wheat-straw based alkyl polyglucoside (APG), via the previously suggested green low-waste generating processes (supercritical CO<sub>2</sub> extraction, low-temperature microwave and in-situ fractionation of platform chemicals). A wheat straw-derived APG production pathway was compared economically to palm-kernel and wheat-grain APG. Total processing costs were determined to range between \$0.92- \$1.87 per kg of wheat straw-APG, demonstrating relatively better output service quality and energy efficiency, while conventional APG costs \$1.95-\$2.87 per kg,





# Encapsulation of active materials for energy applications

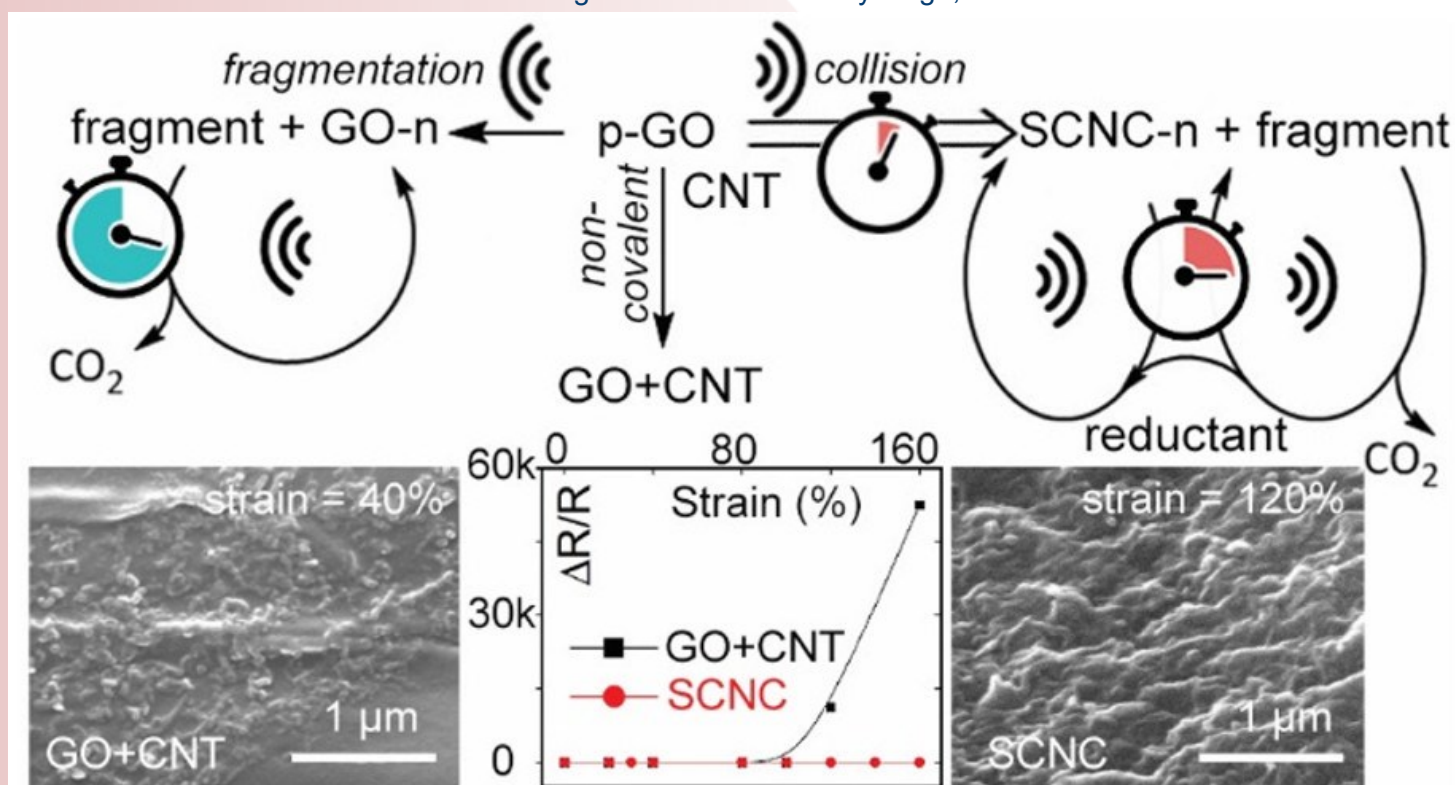
Dmitry Shchukin

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: Unusual Sonochemical Assembly between Carbon Allotropes for High Strain-Tolerant Conductive Nanocomposites

Facile methods toward strain-tolerant graphene-based electronic components remain scarce. Although being frequently used to disperse low-dimensional carbonaceous materials, ultrasonication (US) has never been reliable for fabricating stretchable carbonaceous nanocomposites (SCNC). Inspired by the unusual sonochemical assembly between graphene oxide (GO) and carbon nanotube (CNT), we verified the roots-like GO–CNT covalent bonding, rather than just  $\pi$ – $\pi$  conjugation, was formed during US. In addition, the shock-wave-induced collision in the binary-component system enables a burst of fragmentation at the early stage,

spatially homogeneous hybridization, and time-dependent restoration of graphitic domains. All these are distinct from extensive fragmentation of a conventional single-component system and  $\pi$ – $\pi$  conjugative assembly. The optimized SCNC exhibits conductivity comparable to reduced monolayer GO and outperforms  $\pi$ – $\pi$  assemblies in retaining electrical conductance at a strain of 160%—among one of the best reported stretchable conductors. Raman analysis and mechanics simulation confirm the dominant role of counterweighing between the intrinsic and external strains on the mechano-response and durability of SCNC. This work suggest guidelines for creating multiple-component sonochemical systems for various functional nanocomposites.



US-assisted formation of GO–CNT covalent bonds: Schematic representation shows the formation procedure of SCNC-n, GO + CNT, and GO-n (top). SEM images of SCNC-15 flakes deposited on a PDMS substrate which was stretched by a precise vice and resistance of SCNC-15.

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# Homogeneous catalysis and organometallic chemistry for organic synthesis

## Alexey Sergeev

We focus on improving existing and discovering new catalytic reactions for the synthesis of value added chemicals and fuels from non-renewable (petroleum, coal) and renewable (lignin) natural resources under mild temperatures and with minimum side products. We investigate the key steps underpinning these reactions, that is, activation of the most abundant, yet relatively inert, C-H, C-C and C-O bonds using well-defined metal complexes. We investigate both reactivity and mechanisms of these processes using a combination of experimental methods (NMR, GC, GC-MS, HR-MS and XRD), and theoretical computations (DFT) in collaboration with our colleagues from University of Liverpool and University College of Dublin.

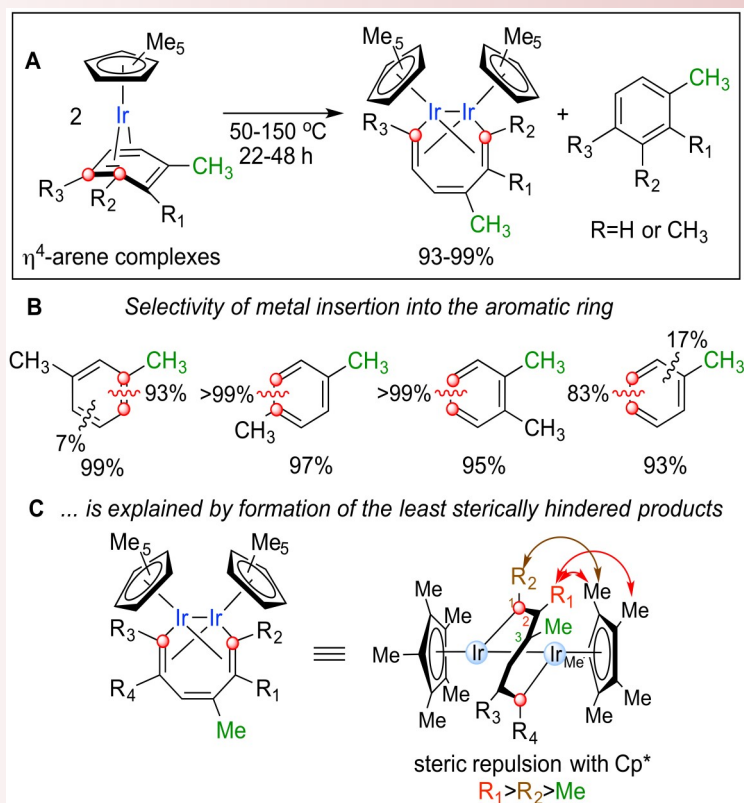
**Highlight: Reversible insertion of iridium into arene ring C-C bonds with improved regioselectivity at a higher reaction temperature.**

Cleavage of the arene ring is the fundamental transformation underpinning conversion of coal and petroleum-based aromatic hydrocarbons into fuel and bulk chemicals. Transition-metal catalysts facilitate this cleavage, but high temperatures (>300 °C) are usually needed and complex mixtures of products are produced. We developed iridium-based system that cleaves

aromatic rings of the most common industrial arenes under much milder temperatures (50-150 °C) to give valuable metallacycle products in nearly quantitative yields. Equally important, iridium cleaves only specific C-C bonds of the substituted aromatic ring and the direction of the cleavage can be predicted using a simple rule. Making this reaction catalytic would lead to much

milder, cleaner and safer processes for converting aromatic hydrocarbons and fossil fuel into key industrial chemicals.

Jakoobi, M.; Sergeev, A. G. Transition-Metal-Mediated Cleavage of C-C Bonds in Aromatic Rings. *Chem. Asian J.* **14**, 2181-2192 (2019).



(A) Insertion of iridium into the aromatic ring of toluene, m-, p- and o-xylenes, (B) regioselectivity of the insertion; (C) key steric interactions determining the relative stability of the metallacycle products and observed selectivity of the insertion. Published under a Creative Commons Attribution License in *J. Am. Chem. Soc.* **141**, 6048-6053 (2019)

# Semiconductor Material Physics for Renewable Energy

## 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 characterization of semiconductors enables the development new advanced materials and understanding for future sustainable energy technologies. Particular current focusses include novel dopants in transparent con-

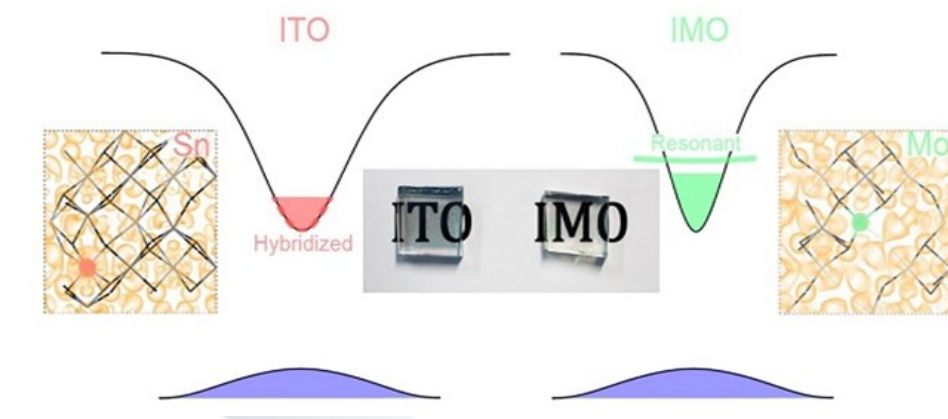
ducting oxides, ultra-thin metal layers as transparent conductors, new photovoltaic absorber materials and band alignment measurement and design in solar cells.



## Highlight: Resonant transition metal donors for high mobility transparent conductors

Tin doped indium oxide – ITO – is the leading transparent conductor for touch screens, solar cells and light emitting diodes because it conducts electricity and allows light through. ITO accounts for 60 per cent of the multibillion dollar transparent conducting oxide market and 60 per cent of global indium use. The search for materials that can replace ITO has increased significantly in recent years, as supplies of indium decrease and its price significantly increases.

In our work, a combination of experimental and theoretical approaches have been used to explain how replacing tin with the transition metal molybdenum creates a vastly superior material – IMO – that has twice the conductivity of ITO. It can deliver



Schematic representations of the conduction band dispersion of ITO where Sn 5s states mix strongly with the In 5s host states and of IMO where Mo 4d states mix minimally with the In 5s states. Partial charge density at the conduction band minimum is also shown from density functional theory. Published under a Creative Commons Attribution License in J. E. N. Swallow *et al.*, *Materials Horizons* **7**, 236-243 (2020)

better performance than ITO with only half the thickness and half the amount of indium. Although IMO was first made several years ago, the reasons why it is so much better than ITO were not understood. This

research enables a reduction of indium use in displays and touch screens and also provides a route for better, cheaper earth-abundant transparent conductors for renewable energy applications.

## Energy conversion in molecular devices

### Andrea Vezzoli

Molecular nanotechnology offers exciting advantages for the fabrication of devices with low power consumption and low toxicity, alongside a tremendous reduction in size and the attractive possibility of integration in printed devices and flexible electronics. The use of molecules as energy converters further opens up the possibility of exploiting quantum effects to attain high efficiency: quantum interference can yield high thermal conversion, and quantum confinement results in exceptional photonic phenomena.

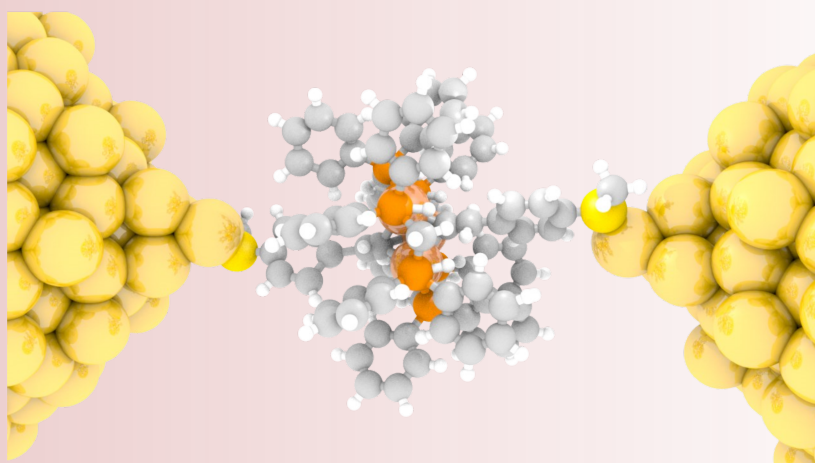
Our approach, relying on a combination of chemical synthesis and physical measurements enables the development of novel device architectures, while studying fundamental quantum phenomena at the smallest scale possible.

### Highlight: Single-entity Electronics and Photonics of Chemically Wired Nano-crystals

The project aims at developing light sources operating at the nanoscale. At this extremely reduced scale, matter behaves in novel ways,

following the rules of quantum mechanics.

Exploiting these rules and a resulting phenomenon called quantum confinement, crystals of nanometre size exhibit surprising light-emission properties. By chemically wiring one of these crystals to two nanoelectrodes, we aim at developing efficient single-photon emitters for their use in power-hungry fields such as sensors, quantum optics and quantum cryptography.



Example of a molecular device. A copper-phosphino nanocluster (orange) is chemically wired to two gold nanoelectrodes by organic ligands (grey).

# SIRE building strong links with China

SIRE has forged strong collaborative links with leading Physical Chemistry Laboratory at Xiamen University China. Four SIRE academics (Profs Cowan, Dhanak, Hardwick and Shchukin) have recent joint publications with Xiamen collaborators (see

box) following a sustained series of research exchanges and academic visits over the past 5 years. Royal Society travel grant and university seed funding has supported this long-term interaction with Tom Galloway, Julia Vidal-Fernandez, Khezar

Saeed and Mark Forster spending research time in Professor Jian-Feng Li's laboratories in Xiamen. Jin-Chao Dong and Yao-Hui Wang have both had 3-month research visits to Professor Hardwick's group in SIRE.

K. H. Saeed, M. Forster, J. F. Li, L. J. Hardwick, and A. J. Cowan, Water oxidation intermediates on iridium oxide electrodes probed by in situ electrochemical SHINERS. *Chem. Commun.* **56** (2020) 1129-1132.

T. A. Galloway, J. C. Dong, J. F. Li, G. Attard and L. J. Hardwick, Oxygen reactions on Pt{hkl} in a non-aqueous Na<sup>+</sup> electrolyte: Site selective stabilization of a sodium peroxy species, *Chem. Sci.* **10** (2019) 2956-2964.

Z. Zheng, J. Jin, J. C. Dong, B. Li, G. K. Xu, J. F. Li, D. G. Shchukin, Unusual Sonochemical Assembly between Carbon Allotropes for High Strain-Tolerant Conductive Nanocomposites, *ACS Nano* **13** (2019) 12062-12069.

D. W. Davies, A. Walsh, J. J. Mudd, C. F. McConville, A. Regoutz, J. M. Kahk, D. J. Payne, V. R. Dhanak, D. Hesp, K. Pussi, T.-L. Lee, R. G. Egdell and K. H. L. Zhang, Identification of Lone-Pair Surface States on Indium Oxide, *J. Phys. Chem. C* **123** (2019) 1700-1709.

J. Y. Zhang, W. W. Li, R. L. Z. Hoyer, 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** (2018) 2275-2282.



## ECS Northwest Student Chapter Conference

On November 27<sup>th</sup> 2018, The Electrochemical Society (ECS) Northwest Chapter organised a student-lead conference held in Stephenson Institute for Renewable Energy, University of Liverpool (UoL), UK. The conference saw over 40 students and academics from the Universities of Liverpool, Manchester, Lancaster, Chester, Bath and Bristol coming together to share knowledge and ideas about all things electrochemistry. Guest speaker Prof. Frank Marken from the University of Bath gave a talk entitled: 'Electrochemistry within Polymers of Intrinsic Microporosity'. The talk was informative and the chapter hopes to welcome Frank back in the future to give more talks on his area of research.

The conference also included a series of talks given by our student and academic members: Charlotte Smith from UoL gave a talk on *Perylene bisimide gels for their use in photoelectrodes*; Dr David Ward

from the University of Chester presented on *Temperature and catholyte concentration effects within regenerative redox fuel cells*; Khezar Saeed from UoL presented on *In-situ surface sensitive vibrational spectroscopy of (photo)-electrodes*; prize winner Gaël Gobaille-Shaw presented on *CO<sub>2</sub> conversion to methanol at very low overpotential on Pt-Fe alloys*; and finally Dr Alex Cowan from the UoL gave an illuminating talk as the internal speaker entitled: '*In-situ studies of electrode surfaces during catalytic CO<sub>2</sub> reduction*'. All of our presenters provided interesting talks and gave us the opportunity to experience and appreciate each other's research, helping strengthen the research ties between our North Western institutes.

The event also included a poster session and was concluded with an award ceremony where sponsors Alvatek and Metrohm presented awards for best talk and best poster.

This year's prize winners (pictured below) were: Gaël Gobaille-Shaw from the University of Bristol, and Jack Beane from UoL, respectively.



Prof Frank Marken giving his talk.



# PhD Theses in 2018/19



Dr Nikolas Antonatos  
Adsorbates on Metal  
Single Crystal Electrodes  
Supervisors: Yvonne  
Gründer, Chris Lucas,  
David Martin



Dr Filipe Braga Nogueira  
Electrochemical testing  
of alkali metal-oxygen  
batteries  
Supervisor: Laurence  
Hardwick



Dr. Nick J. Brownbill  
DNP Enhanced NMR of  
Low Abundance, Low  
Gamma and Difficult to  
Observe Nuclei  
Supervisor: Fred Blanc



Dr Jose Coca-Clemente  
Electrochemical and sur-  
face study of lithium-rich  
transition metal oxides  
Supervisors: Laurence  
Hardwick and Vin Dhanak



Dr Joshua Fogg  
Au(hkl) Surface XRD  
at the Electro-  
chemical Interface  
Supervisors: Chris  
Lucas and Yvonne  
Gründer



Dr James Gibbon  
Band alignments and  
interfaces in kesterite PV  
Supervisors: Vin  
Dhanak, Tim Veal and  
Richard Potter



Dr David Vega  
Herrera  
Catalytic upgrading  
of pyrolysis oils  
Supervisor: Tony  
Lopez-Sanchez



Dr Martin Jakoobi  
Ir in the arene ring in  
eta-4-arene complexes  
Supervisors: Alexey  
Sergeev and Gilberto  
Teobaldi



Dr Liqaa Majdal  
Zeolites and  
Advanced Nano-  
materials  
Supervisor: Tony  
Lopez-Sanchez



Dr Silvia Mariotti  
Hybrid and inorganic  
plumbo-halide perov-  
skites for solar cells  
Supervisors: Ken  
Durose and Jon Major



Dr Stefano Mensa  
Modelling and theory of  
polaron trapping in glucose  
based bio-insulators: the  
cyclodextrin case  
Supervisor: Gilberto  
Teobaldi



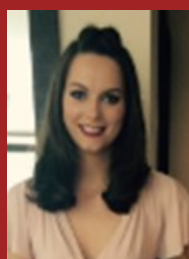
Dr Marios Michailidis  
Nanocomposite Coatings  
for Antibacterial/  
Antifouling Applications  
Supervisor: Dmitry  
Shchukin



Dr Petar Radjenovic  
Ionic Liquid Electro-  
lytes for Non-Aqueous  
Li-O<sub>2</sub> Batteries  
Supervisor: Laurence  
Hardwick



Dr Lena Reichenbach  
Effects of temperature  
on gold single crystal  
electrochemistry  
Supervisors: Yvonne  
Gründer and Chris Lucas



Dr. Charlotte Smith  
Polymer Materials  
for Solar Fuel  
Generation  
Supervisor: Alex  
Cowan



Dr. Jessica Stoner  
Strongly Correlated  
Perovskites  
Supervisor: Jon Alaria



Dr Edgar Yañez  
Supported Metal Nano-  
particles for The Selective  
Transformation of Bio-  
derived Molecules  
Supervisor: Tony Lopez-  
Sanchez



Dr. Peter J Yates  
Emerging absorber  
materials for sustaina-  
ble photovoltaics  
Supervisors: Ken  
Durose and Jon Major

# Publications in 2019

## Jonathan Alaria

I. Marković, C. A. Hooley, O. J. Clark, F. Mazzola, M. D. Watson, J. M. Riley, K. Volckaert, K. Underwood, M. S. Dyer, P. A. E. Murgatroyd, K. J. Murphy, P. Le Fèvre, F. Bertran, J. Fujii, I. Vobornik, S. Wu, T. Okuda, J. Alaria and P. D. C. King  
Weyl-like points from band inversions of spin-polarised surface states in NbGeSb  
*Nature Communications* **10**, 5485 (2019)

J. L. Stoner, P. A. E. Murgatroyd, M. O'Sullivan, M. S. Dyer, T. D. Manning, J. B. Claridge, M. J. Rosseinsky, J. Alaria  
Chemical Control of Correlated Metals as Transparent Conductors  
*Adv. Funct. Mater.* **29**, 1808609 (2019)

## Frédéric Blanc

J. Gamon, B. B. Duff, M. S. Dyer, C. Collins, L. M. Daniels, T. W. Surta, P. M. Sharp, M. W. Gaultois, F. Blanc, J. B. Claridge, and M. J. Rosseinsky  
Computationally Guided Discovery of the Sulfide  $\text{Li}_3\text{AlS}_3$  in the Li–Al–S Phase Field: Structure and Lithium Conductivity  
*Chem. Mater.* **31**, 9699–9714 (2019)

M. Diaz-Lopez, J. F. Shin, Ming Li, M. S. Dyer, M. J. Pitcher, J. B. Claridge, F. Blanc, and M. J. Rosseinsky  
Interstitial Oxide Ion Conductivity in the Lanthanite Structure: Carrier Trapping by Formation of  $(\text{Ga},\text{Ge})_2\text{O}_8$  Units in  $\text{La}_{3-x}\text{Ga}_{5-x}\text{Ge}_{1+x}\text{O}_{14+x/2}$  ( $0 < x \leq 1.5$ ).  
*Chemistry of Materials* **31**, 5742-5758 (2019)

R. Ramos, A. Grigoropoulos, B. L. Griffiths, A. P. Katsoulidis, M. Zanella, T. D. Manning, F. Blanc, J. B. Claridge and M. J. Rosseinsky  
Selective conversion of 5-hydroxymethylfurfural to diketone derivatives over Beta zeolite-supported Pd catalysts in water  
*J. Catalysis* **375**, 224-233 (2019)

N. J. Brownbill, D. Lee, G. De Paepe, and F. Blanc  
Detection of the Surface of Crystalline  $\text{Y}_2\text{O}_3$  Using Direct  $^{89}\text{Y}$  Dynamic Nuclear Polarization  
*J. Phys. Chem. Lett.* **10**, 3501-3508 (2019)

D. Xiao, X. Han, X. Bao, G. Hou, and F. Blanc  
Identification of different carbenium ion intermediates in zeolites with identical chabazite topology via  $^{13}\text{C}$ - $^{13}\text{C}$  through-bond NMR correlations  
*RSC Advances* **9**, 12415-12418 (2019)

## Alex Cowan

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# Research Grants Held 2019-2020

A total of £35M is currently held by SIRE investigators. New grants won in 2019 are highlighted with an asterisk.

## Engineering & Physical Sciences Research Council

|                                                                                                                                             |            |
|---------------------------------------------------------------------------------------------------------------------------------------------|------------|
| Jon Alaria, Ivana Evans (PI, Durham) <i>et al.</i> , Advanced Inorganic Functional Materials: Floating Zone Crystal Growth System           | £401,688   |
| Jon Alaria, Matt Rosseinsky (PI) <i>et al.</i> , Chemical control of function beyond the unit cell for new electroceramic materials         | £742,473   |
| Jon Alaria, Matt Rosseinsky (PI) <i>et al.</i> , Integration of Computation and Experiment for Accelerated Materials Discovery              | £6,650,587 |
| Frédéric Blanc, Applications of Time-Domain Nuclear Magnetic Resonance in Pharmaceutical Sciences*                                          | £21,000    |
| Frédéric Blanc, Connect NMR UK, A National NMR Network for the Physical and Life Sciences*                                                  | £471,000   |
| Frédéric Blanc <i>et al.</i> , Very-High Field NMR in the Physical and Life Sciences at the University of Liverpool                         | £2,000,000 |
| Alex Cowan (PI), Frank Jäckel, Jon Major, James Walsh, Capital Award emphasising support for Early Career Researchers                       | £336,301   |
| Alex Cowan, Spectroscopy-driven Design of an Efficient Photocatalyst for Carbon Dioxide Reduction                                           | £903,680   |
| Alex Cowan, Matt Rosseinsky (PI), Flexible Routes to Liquid Fuels from CO <sub>2</sub> by Advanced Catalysis and Engineering                | £1,804,265 |
| Vin Dhanak, Peter Weightman (PI) and Michele Siggel-King, FLUENCE                                                                           | £630,891   |
| Ken Durose, International Collaboration Activities                                                                                          | £11,000    |
| Ken Durose, Centre for Doctoral Training in New and Sustainable Photovoltaics                                                               | £5,300,000 |
| Ken Durose (PI) and Jon Major, New Designs for Thin Film Solar Cells*                                                                       | £505,552   |
| Yvonne Gründer and Chris Lucas (PI), XMaS: The UK Materials Science Facility at the ESRF                                                    | £3,515,607 |
| Laurence Hardwick, ISCF Wave 1: Earth-Abundant Metal-Air Batteries                                                                          | £1,086,474 |
| Laurence Hardwick, Andy Cooper (PI), Porous Liquids: Understanding, Scope and Applications                                                  | £535,720   |
| Laurence Hardwick, Multi-Scale Analysis for Facilities for Energy Storage (MANIFEST)                                                        | £111,592   |
| Laurence Hardwick (PI), Neil Berry and Richard Nichols, The Calcium-Air Battery                                                             | £251,028   |
| Laurence Hardwick, Alex Cowan and Nigel Browning (PI), Quantitative Imaging of Multi-Scale Dynamic Phenomena at Electrochemical Interfaces* | £410,406   |
| Laurence Hardwick, John Claridge and Matthew Rosseinsky, Next Generation Li-ion Cathode Materials (CATMAT)*                                 | £2,116,284 |
| Laurence Hardwick (PI), John Claridge and Matthew Rosseinsky, SOLBAT- The Solid-State (Li or Na) Metal-Anode Battery                        | £1,462,215 |

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| Laurence Hardwick (PI), Towards a Comprehensive Understanding of Degradation Processes in Electric Vehicle Batteries | £390,015 |
| Frank Jäckel and Richard Nichols (PI), Single-Molecule Plasmoelectronics                                             | £444,776 |
| Tony Lopez-Sanchez and Jianliang Xiao (PI) Iron-Catalysed Oxygenation with O <sub>2</sub>                            | £349,398 |
| Jon Major, Capacitance Spectroscopy Led Process Innovations to Improve V <sub>OC</sub> in CdTe Thin Film Solar Cells | £810,102 |
| Alexey Sergeev (PI), New Functionalisation of Arenes Through Metal-Mediated Scission of Strong Aromatic C-C Bonds*   | £121,770 |
| Tim Veal (PI) and Vin Dhanak, Donor Design for Maximum Mobility TCOs                                                 | £509,182 |

## Royal Society

|                                                                                                           |          |
|-----------------------------------------------------------------------------------------------------------|----------|
| Yvonne Grunder, Electrochemical modification and Deposition of Bifunctional Metal-alloys and Metal-oxides | £329,024 |
| Laurence Hardwick, Understanding Oxygen Reduction and Evolution Reactions Using SHINERS                   | £12,000  |
| Andrea Vezzoli, Single-entity Electronics and Photonics of Chemically Wired Nanocrystals*                 | £770,086 |

## Leverhulme Trust

|                                                       |          |
|-------------------------------------------------------|----------|
| Alex Cowen, Gel-Based Photoelectrodes for Clean Fuels | £125,987 |
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## Industry

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| Frédéric Blanc, Bristol-Myers Squibb: Solid-State NMR of Amorphous Spray Dried Dispersions | £80,000 |
| Tim Veal (PI), Vin Dhanak and Jon Major, NSG Group, Interface Electronic Properties        | £12,000 |

## Innovate UK

|                                                                  |          |
|------------------------------------------------------------------|----------|
| Laurence Hardwick, G-Cap Supercapacitor in All-Terrain Vehicles* | £223,801 |
| Laurence Hardwick, Practical and Robust Lithium Air Batteries    | £137,300 |

## European Commission

|                                                                                                                |          |
|----------------------------------------------------------------------------------------------------------------|----------|
| Alex Cowan, SEAFUEL                                                                                            | £269,486 |
| Ken Durose, INDEED - Innovative Nanowires Device Design                                                        | £308,208 |
| Dmitry Shchukin, ENERPAINT - New thermo-regulating paints based on nanoencapsulation of phase-change materials | £135,000 |

## UK-India Education & Research Initiative British Council

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| Vin Dhanak and Ivona Mitrovic, Dielectric Engineering on GaN for Sustainable Energy Applications | £50,000 |
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# SIRE Staff Directory

| Name                                                      | Email                    | Telephone             | Subject                                      |
|-----------------------------------------------------------|--------------------------|-----------------------|----------------------------------------------|
| Alaria, Dr Jonathan                                       | alariaj@liverpool.ac.uk  | +44 (0)151 794 3366   | Oxides, magnetic and thermoelectrics         |
| Blanc, Dr Frédéric                                        | fblanc@liverpool.ac.uk   | +44 (0)151 794 3511   | NMR spectroscopy                             |
| Cowan, Prof Alexander<br>EPSRC Research Fellow            | acowan@liverpool.ac.uk   | +44 (0)151 794 3481   | Electro and photo catalytics conversion      |
| Dhanak, Prof Vin                                          | vin@liverpool.ac.uk      | +44 (0)151 795 0534/1 | Electronic structure of advanced materials   |
| Durose, Prof Ken                                          | dph0kd@liverpool.ac.uk   | +44 (0)151 795 9048   | PV materials and devices                     |
| Gründer, Dr Yvonne<br>Royal Society Research Fellow       | grunder@liverpool.ac.uk  | +44 (0)151 795 2156   | Fundamental electrochemistry                 |
| Hasell, Dr Thomas<br>Royal Society Research Fellow        | t0m@liverpool.ac.uk      | +44 (0)151 794 3502   | Sulfur polymers and functional materials     |
| Hardwick, Prof Laurence<br>Director                       | hardwick@liverpool.ac.uk | +44 (0)151 794 3493   | Batteries and electrochemistry               |
| 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<br>EPSRC Research Fellow                    | jonmajor@liverpool.ac.uk | +44 (0)151 795 9049   | PV materials and devices                     |
| Mumtaz, Dr Asim<br>Lecturer and Academic Manager - CDT-PV | amumtaz@liverpool.ac.uk  | +44 (0)151 795 7565   | PV materials and devices                     |
| Sergeev, Dr Alexey                                        | sergeev@liverpool.ac.uk  | +44 (0)151 794 2665   | Novel catalytic transformations              |
| Shchukin, Prof Dmitry                                     | shchukin@liverpool.ac.uk | +44 (0)151 795 2304   | Nanoencapsulation                            |
| Veal, Prof Tim                                            | timveal@liverpool.ac.uk  | +44 (0)151 794 3872   | Semiconductor materials and physics          |
| Vezzoli, Dr Andrea<br>Royal Society Research Fellow       | skeja@liverpool.ac.uk    | +44 (0)151 795 3128   | Molecular technologies for energy conversion |





UNIVERSITY OF  
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## Contact

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

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

T: +44 (0)151 795 8137

E: [sire.support@liverpool.ac.uk](mailto:sire.support@liverpool.ac.uk)



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