UNIVERSITY OF LIVERPOOL

Stephenson Institute for Renewable Energy

Annual Reports 2020 and 2021

LIFE CHANGING
World Shaping

The Stephenson Institute for Renewable Energy Report: 2020 and 2021

Contents

The Annual Report 2020 and 2021 was collated and edited by Tim Veal and Ken Durose

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

Director’s Welcome

Welcome to the SIRE Report for 2020/21 - a snapshot of our work on the chemistry and physics of energy storage, conversion 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, SIRE exploits the research expertise on technologies such as solar energy, solar fuels, batteries, electrolysers and electrochemical capacitors.

As we are all aware 2020 and 2021 was a challenging time and I would like to commend how well everyone pulled together and worked through this period. It is impressive how much amazing science was still carried out, which you can read the highlights of in this report.

It has been another busy period for PhD graduations. Twenty-six of our early stage research colleagues successfully defended their theses in 2020 and 2021:
Tom Baines, Daniel Cheung, Tom Featherstone, Claudia Gatti, Theo Hobson, Sophie Hodgkiss, Ashlea Hughes, Kenneth Inglis, Xiaochen Liu, Javier Mejía, Phil Murgatroyd, Graeme O’Dowd, Romen Padila, Douglas Parker, Robyn Presland, Samuel Petcher, Verity Piercy, Tom Shalvey, Huw Shiel, Jessica Smith, Jack Swallow, Siti Supardan, George Wilson, Dong Xiao, Ruowei Yi and Xiaolei Zhu.

Their thesis titles and photos appear towards the end of this report. Everyone 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 on page 34.

Laurence Hardwick,
SIRE Director

Impact and Events

The Solar Fuels Network led by The University of Liverpool

The Solar Fuels Network (SFN) represents more than 550 members drawn from the across the UK's solar fuels academic and industrial research community. The management of the SFN has recently transferred from Cambridge University to Liverpool with Professor Alex Cowan taking on the Directorship and it is based at the Stephenson Institute for Renewable Energy.

Solar Fuels and chemicals are generated from abundant molecules (e.g. water, carbon dioxide, nitrogen) using sunlight as the energy source. Producing energy rich fuels such as (green) hydrogen, methanol and even gasoline using solar energy is an attractive goal as it offers a way to overcome the intermittency of renewables and provides drop in alternatives to fossil derived products for heating and transportation sectors that are hard to electrify (e.g. aviation).

The SFN aims to develop an effective community of solar fuels researchers from both academia and industry. It seeks to raise the profile of the UK solar fuels research community nationally and internationally, to promote collaboration and cooperation with other research disciplines, industry and international solar fuels programmes, and to contribute towards the development of a UK solar fuels technology and policy roadmap.

A key role of SFN is to help bring together the many perspectives, disciplines and challenges facing renewable solar energy today, working to achieve a cost effective and renewable synthesis of molecular fuels.

SFN supports various activities and events and works closely with partner organisations including the Royal Society of Chemistry, the Energy community of the Knowledge Transfer Network, the Solar Fuels Institute and the Foreign and Commonwealth Office's Science and Innovation Network.

Activities include the organisation of workshops and conferences, post graduate symposia, public engagement events, and the publication of a regular newsletter. Membership is free and available to both UK-based and international researchers. Membership gives access to events, workshops and seminars related to solar-driven fuels synthesis, and members receive a quarterly newsletter. Bursaries are available for UK-based members for travel, outreach and public engagement, and bilateral exchange.

Full details of the Network, Membership and events can be found on its web site https://www.solarfuelsnetwork.com/.

SFN's 8th Symposium

On December 1st 2020 the delayed 8th UK Solar Fuels Network Symposium was held online. The meeting was planned to be held in person at the University of Liverpool in the spring but it was decided to move online once the severity of the COVID outbreak became clear. Although we missed the chance to meet colleagues in person, as is often the case, there was a silver-lining.

Typically, SFN in-person symposia attract around 100 people, in contrast we had over 230 individuals join our online webinar. We were particularly excited to see the global reach of the event with people logging in from over 30 different countries from 6 different continents (come on Antarctica you are letting the side down!). Registrants heard a fantastic range of presentations from our invited speakers and we are incredibly grateful to Professors Roel van de Krol, Andy Cooper, Erwin Reisner, Andrew Mills and Dr Ludmilla Steier.

This great experience has led the SFN advisory board to decide that going forward we will aim to run SFN symposia as hybrid events with both in person and online registration to maximise accessibility. If you are reading this from the British Antarctic Survey there is no excuse next time- let's get all 7 continents involved in solar to fuels!

Joint SFN/SuperSolar Early Career Researchers Meeting

A joint online early career researcher's (ECR) meeting was organised by Solar Fuels Network and SuperSolar and hosted by Imperial College London. This online webinar was attended by some 90 people from across the world.

The meeting was split into two sessions one for each of the networks with an introduction from Professor Michael Walls (SUPERGEN, Loughborough University). Session one was chaired by Dr Anna Hankin of Imperial with a keynote from SIRE's very own Dr Jon Major (University of Liverpool) who presented 'Antimony Selenide Thin Films for Photovoltaics and Photoelectrochemical Water Splitting'. ECR presentations were given by Rajiv Prabhakar (University of Zurich); Tamara McFarlane (Swansea University); Flurin Eisner (Imperial College London) and Isaac Holmes-Gentle (Swiss Federal Institute of Technology Lausanne).

In session two, chaired by Dr Ludmilla Steier from Imperial, a keynote was given by Dr Qian Wang, (University of Cambridge) 'Scalable Photocatalyst Sheet for Artificial Photosynthesis'. This was followed by ECR presentations from Ibbi Ahmet (Helmholtz-Zentrum Berlin); Adriana Augurio (Queen Mary University of London) and Cui Ying Toe (University of New South Wales). The sessions generated lots of great questions and it was fantastic to hear from the ECR's of these two closely aligned fields.

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

The Centre for Doctoral Training in New and Sustainable Photovoltaics (CDT-PV) is a multicentre team composed of seven universities - Liverpool, Bath, Sheffield, Loughborough, Southampton, Oxford and Cambridge. The CDT-PV is a UK national centre that has 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 - and hence significantly contribute towards net zero carbon emission targets. These solar cells will need to be made from the new and sustainable materials that are the focus of our research and training. The seven partner universities give the Centre to have thorough coverage of the research themes and training needs relevant to the future of solar electricity generation.

Despite the immense challenges of Covid-19, we were very pleased that majority of our third cohort of doctoral students were able to successfully complete their PhDs. We are extremely proud that many of the graduates across our first three cohorts from the centre have decided to continue to pursue research in photovoltaics through post-doctoral/academic roles and also jobs within the industry. As well this we are pleased that graduates have entered wider sustainable technology fields in both research and industry, as well in the field of policy.

The centre has had a total of 60 students with 44 supervising academics across the seven partner universities. The students from the Centre continue to produce high quality work which has been presented at a number of the leading international photovoltaic conferences and published in high ranking journals (www.cdt-pv.org/publications/). The students also remain actively engaged in fantastic outreach work related to science/photovoltaics, both to schools and local communities.

Training Events in 2020/2021

In early 2020 a training event was held for the CDT-PV students at the University of Liverpool in London Campus. This event was organised specifically for our last three cohorts 3, 4 and 5 students. The event was held over two days, with the first day focussed on careers. A range of speakers from different sectors were invited to deliver talks on their career's paths. Speakers from publishing, consultancy, civil service, patent law and academia were all present. Kerry Hayes from Regen SW spoke about her career path and the activities she was involved in as a renewable energy consultant. Dr Piers Barnes from Imperial College London spoke about his experiences and route into academia.

Continued...

CDT-PV (Continued)

Other speakers were Dr Elisa De Ranieri (Editor in Chief, Nature Communications), Jenni Penrose (Civil Service, Government Science and Engineering Profession), Dr David Grant (Marks & Clerk Patent Attorney), Dr Chris Punshon (TWI Power Industry Sector Manager) and Imogen Small (Institute of Physics Outreach team). Each talk was followed by a lively question and answer discussion. A poster session was organised for the students, which gave a nice opportunity for the student to present updates in their projects and learn about developments across the centre. Best poster prizes were awarded to Alan Bowman (Cambridge) and Kaya Bretchley (Bath). Members of the Centre for Doctoral Training in Plastic Electronics were also invited to the event.

On the following day there was a focus on specific academic topics that were of interest to the students. These included a talk on 3D Photovoltaic Modelling delivered by Dr Tasmiat Rahman from the University of Southampton. Dr Jenny Clark from the University of Sheffield gave a talk on Spectroscopy of organic photovoltaics. There was another talk entitled “Moving beyond spin-coating; progress and challenges in printing perovskites” presented by Professor Trystan Watson from SPECIFIC at Swansea University. Professor Daniel Wolverson from the University of Bath delivered a talk on the Carrier resolved Photo-Hall Effect. The last talk of the event was by Jennifer Steven, Careers Consultant at Skillfluence Ltd, who spoke about CV writing, interview preparation and transferrable skills.

Location for the CDT-PV 2020 Winter Training Event

As a consequence of the pandemic other training events this year were held online. An online event was organised for the students, about “How to manage your PhD to minimise Covid-19 impact”. The event was delivered by Dr Lisa Cox from Life Compass consulting who had specially developed this course for doctoral students.

A “Research Roundtable” event was held for each of the cohorts, where students had an opportunity to present an update on their research projects. We also used the opportunity to get the students to discuss what they saw as the biggest challenges they are facing and what support/training would be really helpful in the coming months/years. These answers to these questions will feed into future planned events.

As a consequence of the feedback, another online careers event was held with three excellent speakers, two on academic career paths and one about the UK solar industry. We are now fortunate that our earlier cohorts have graduated and are all progressing in a variety of careers. Dr Juliane Borchert from our second cohort delivered an excellent talk on her experiences towards the end of her PhD in searching for a job and in securing her first research position. Her thoughts and practical advice were extremely beneficial to students. Other speakers included Dr Michael P. Weir from the School of Physics and Astronomy at the University of Nottingham, who spoke about Post-PhD careers, sharing his experience, thoughts and advice, over the 10 years since he graduated with a PhD and securing permanent academic post. Finally, Will Hitchcock, CEO and Founder of Above Surveying, who presented his experiences in moving from the corporate IT world to pioneering aerial inspection techniques in utility scale solar farms. All talks very well received by the students who asked a range of questions, which kept the post presentation discussions very engaging.

Dr Asim Mumtaz

Lecturer & Deputy Director CDT-PV

Kerry Hayes from Regen SW speaking about her career path and her work as a renewable energy consultant

CDT-PV Leadership

The CDT-PV was the brain child of Professor Ken Durose, who while Director of the Stephenson Institute, who led the submission of the CDT-PV as well as leading the Centre since its inception in 2014. The Centre was one of the first of its kind being based on a distributed partner model, the first CDT in Liverpool, and a successful model which other centres now follow. In late 2020, Professor Ken Durose had to step down due to personal reasons, after having led the Centre successfully for 6 years.

In recognition of his efforts in establishing and leading the centre, as well developing the community, many students past and present as well as academics kindly donated a card and gifts of appreciation. Since then Professor Alison Walker from the University of Bath was appointed as Director and Dr Alan Dunbar from University of Sheffield was selected as the Academic Director of the centre, to continue the training efforts. Dr Asim Mumtaz continued as Deputy Director.

Prof Ken Durose receiving a gift from the students and staff of the CDT-PV after stepping down

Research Group Expertise and Highlights

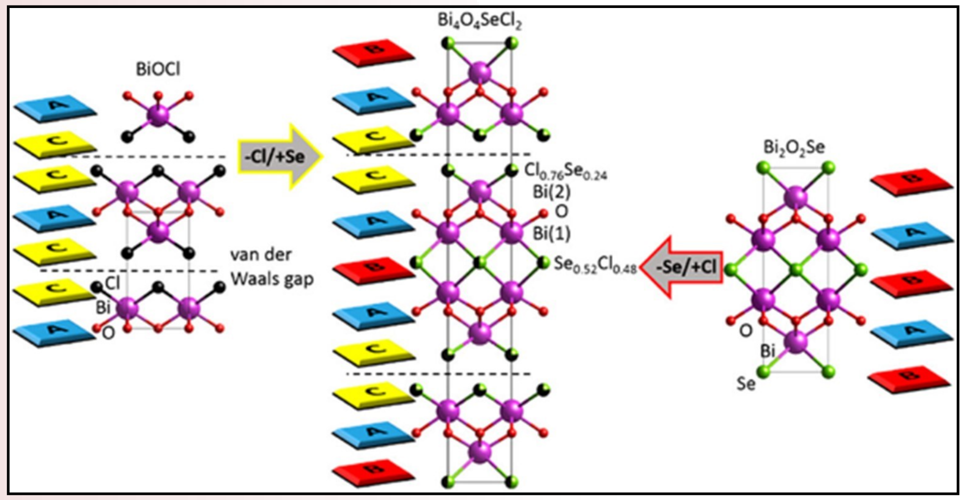
Crystal growth, magnetism and thermoelectrics

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 with important physical properties or applications in renewable energy. Physics understanding and methodologies (such as quantum oscillations) are combined with chemistry know-how and intuition. Our main focus in renewable energy materials is the design of novel ways to break the conventional interdependence of thermal and electronic conductivity in order to develop improved thermo-electric materials.

Highlight: Modular Design of High Mobility van der Waals Semiconductor $Bi_4O_4SeCl_2$

Making new van der Waals materials with electronic or magnetic functionality is a chemical design challenge for the development of two-dimensional nanoelectronic and energy conversion devices. The synthesis and properties of the van der Waals material $Bi_4O_4SeCl_2$ is presented. The presence of three anions gives the new structure both the bridging selenide anion sites that connect pairs of Bi_2O_2 layers in Bi_2O_2Se and the terminal chloride sites that produce the van der Waals gap in BiOCl. This retains the electronic properties of Bi_2O_2Se while reducing the dimensionality of the bonding network connecting the Bi_2O_2Se units to allow exfoliation of $Bi_4O_4SeCl_2$ to 1.4 nm height.



*Comparison of the crystal structures of BiOCl, Bi_2O_2Se and $Bi_4O_4SeCl_2$. Published under a Creative Commons Attribution License in Q. D. Gibson et al., J. Am. Chem. Soc. **142**, 847–856 (2020). Copyright 2020 American Chemical*

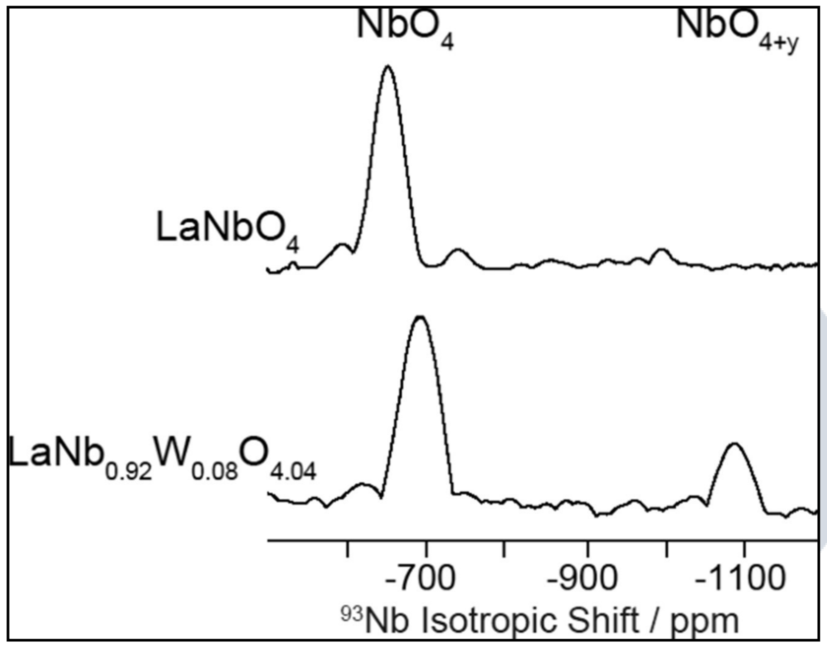
Magnetic resonance for energy materials and catalysis

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: Evolution of structure in the incommensurate modulated $LaNb_{1-x}W_xO_{4+x/2}$ (x = 0.04–0.16) oxide ion conductors

Hyper-stoichiometric $CeNbO_{4+d}$ phases demonstrate remarkable oxygen diffusivity and provide an interesting structural template for oxygen ion conductors. Previously, we have reported the room temperature structure of the incommensurate modulated $LaNb_{0.88}W_{0.12}O_{4.06}$, a structural analogue of $CeNbO_{4+d}$. We confirmed that it is a pure oxygen ion conductor, with anions diffusing via an interstitialcy mechanism. However, the high temperature structural information for the $LaNb_{1-x}W_xO_{4+d}$ (x = 0.04–0.16) family, key to understanding the structure–property relationship in oxygen ionic conductors with complex structures at operating conditions, is unreported. Here, we address this by investigating the high temperature structural evolution of the $LaNb_{1-x}W_xO_{4+x/2}$ phases using a combination of thermal analysis, scattering techniques, and ^{17}O and ^{93}Nb nuclear magnetic resonance spectroscopy (see figure). We reveal a series of phase transitions between a modulated monoclinic phase, a high temperature modulated tetragonal phase, and a high temperature unmodulated tetragonal phase. These findings are correlated with the ion transport and offer insights into the design of new materials for solid state electrochemical devices.



*Projection of the isotropic dimension of the ^{93}Nb triple quantum magic angle spinning (MAS) NMR spectra of $LaNbO_4$ and $LaNb_{0.92}W_{0.08}O_{4.04}$ obtained at room temperature at 20 T and under a MAS rate of 78 kHz. The positions of the Nb sites in tetrahedral symmetry (NbO_4) were tentatively attributed to the niobium environment (NbO_{4+y}, y > 1) with coordination larger than four. Reprinted with permission from Cheng Li et al., Chem. Mater. **32**, 2292–2303 (2020). Copyright 2020 American Chemical Society.*

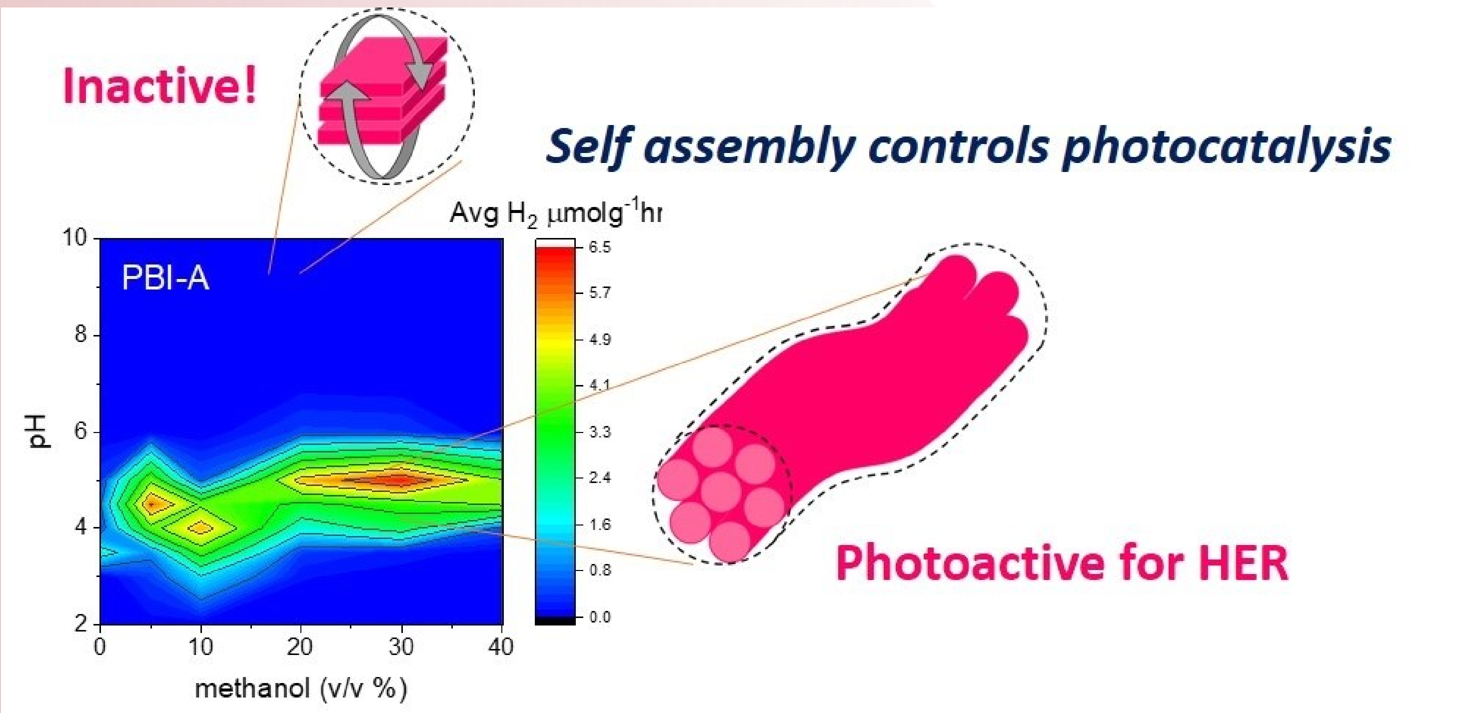
Sustainable and solar fuels

Alex Cowan

We develop and study 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. A recent focus has been on the chemistry of carbon dioxide utilisation with programmes studying both light driven and electrochemical catalysts that can convert waste carbon dioxide into useful chemical feedstocks and fuels. We are also developing new catalysts for water oxidation that can operate in low grade/sea water and light driven catalysts for hydrogen evolution from water. Part of our work is to study the mechanisms of the catalysts using laser based techniques such as vibrational sum-frequency generation spectroscopy.

Highlight: Self-assembled photocatalysts for hydrogen production

Photocatalysts, materials that absorb solar energy to drive a chemical reaction, can be used to generate hydrogen from water. This is an exciting concept that offers a way to generate a storable chemical fuel that can be used to power vehicles and homes from sunlight and water. Historically the research community has tried to improve the activity of photocatalysts by synthetic modification of their chemical structure. This can be a time consuming and costly process. In our work we show how photocatalyst activity can also be controlled by taking a common molecule and assembling it into different larger structures. The small sub-unit is an organic dye known as a perylene bisimide that can self-assemble to form different shapes consisting of many thousands of dye sub-units stacked together. We find that it is possible to trigger self-assembly of an active worm like structure by changing the solvent composition, demonstrating a simple way to make new photocatalysts that can generate hydrogen in water.



The light driven hydrogen evolution rate of an organic photocatalyst depends on the way that the small molecule self-assembles. Self-assembly is directed by the solvent (pH, composition) conditions. Published under a Creative Commons Attribution License in D. McDowall et al., Advanced Energy Materials, 10(46), 2002469, (2020)

Photoemission measurements for advanced functional materials

Vin Dhanak and Tim Veal

We specialise in photoemission measurements of novel advanced materials related to solar conversion and battery storage research as well as gate dielectrics for both low and high-power metal-oxide-semiconductor field-effect transistors. Photoemission (XPS, UPS) and inverse photoemission (IPES) 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 CZTS and related PV absorber materials by chemical bath, spray pyrolysis and magnetron sputter techniques. Additionally, the ultrahigh vacuum systems in our laboratory also have scanning tunnelling microscopy and low energy electron diffraction capabilities for surface structural studies.

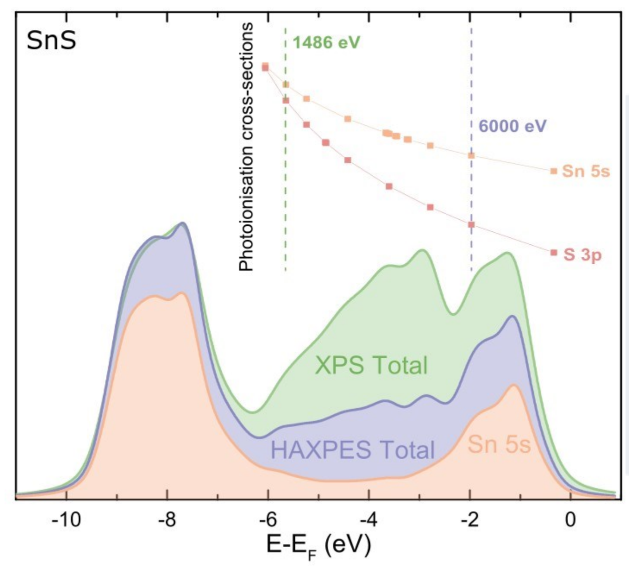
Highlight: Effect of Sn 5s lone-pair states on the electronic structure of tin sulfides

The tin sulfides, like many post transition metal compounds, exhibit two oxidation states where Sn (II) is characterised by an occupied Sn 5s lone pair of electrons which are important for the photoactivity of these materials among other applications in optoelectronics. In XPS and IPES measurements of single crystal SnS, SnS_2 and Sn_2S_3, performed by PhD student Tom Whittles, it was demonstrated that photoemission was a powerful technique to distinguish the different phases of tin sulfides and identifying phase-pure or mixed phase systems [1]. Moreover, comparison of the valence band spectra from XPS and DFT calculations revealed extra states at the top of the valence bands of SnS and Sn_2S_3, arising from the lone pair electrons in Sn (II), which are not present for Sn (IV) in SnS_2, resulting in relatively low ionization potentials for SnS and Sn_2S_3.

To investigate the Sn 5s lone-pair states further, PhD student Leanne Jones used high energy photoemission (HAXPES) at the i09 beamline in Diamond Lightsource, exploiting the different photo-ionization cross sections of the Sn and S orbitals making up the valance band [2]. These new measurements allowed a clearer elucidation of the Sn 5s lone-pair contribution to the electronic structure at the valance band edge of these materials than previously obtained using only soft x-ray photoemission in the laboratory. The results of these papers highlight the advantage of using a combination of photon energies, exploiting the relative photoionization cross sections of the s orbitals with respect to the p orbitals in probing the 5s lone-pair states.

[1] T. J. Whittles et al., Band alignment, valence bands and core levels in the tin sulfides SnS, SnS_2 and Sn_2S_3: experiment and theory, Chemistry of Materials 28 (2016) 3718

[2] L. A. H. Jones et al., Sn $5s^2$ lone pairs and the electronic structure of tin sulfides: A photoreflectance, high-energy photoemission, and theoretical investigation, Phys. Rev. Mater. 4 (2020) 74602.

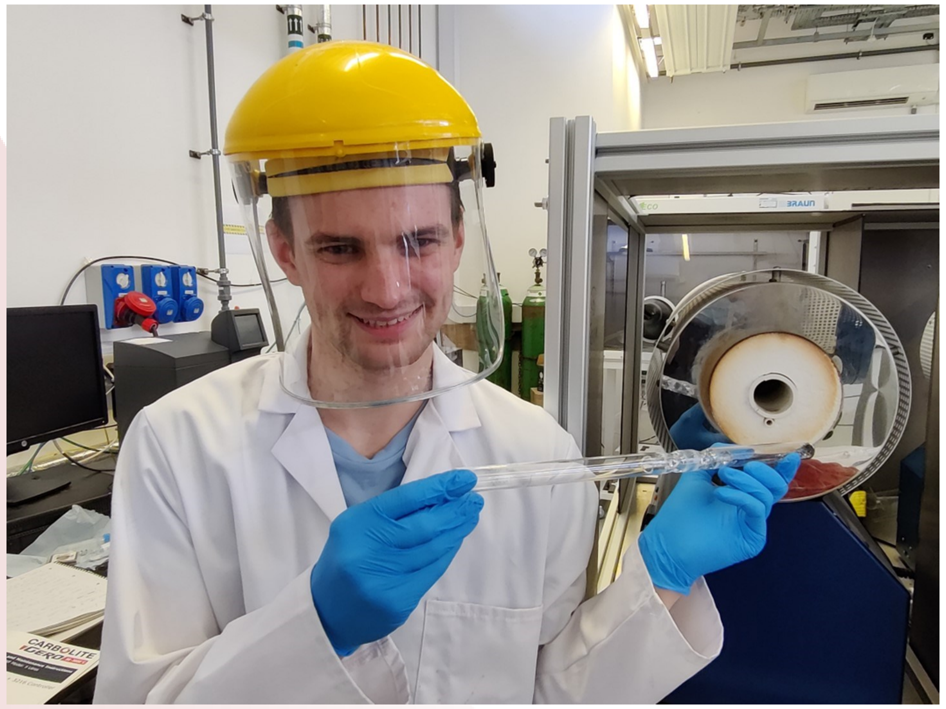


Calculated density of states for Sn 5s (red), compared to measured valence band from HAXPES and lab based XPS from SnS single crystal, highlighting that the majority of the DOS is made up of Sn 5s orbital for HAXPES measurements. Inset shows the calculated photoionization cross sections for Sn 5s and S 3p, indicating that measurements using higher photon energy suppresses the contribution from S 3p.

Single crystals for basic studies of PV materials

Ken Durose

Ken's group researches new types of solar photovoltaic materials and devices that are not yet available commercially. The aim is to enable the solar electricity generating technologies of the future. To achieve the lowest costs, the emerging solar materials are produced in the form of thin film microcrystalline semiconductors - rather than the more expensive single crystalline silicon material used in conventional solar panels. However, while they are cheaper, these thin polycrystalline films give some challenges: for example, the grain boundaries in the films make it difficult or impossible to measure the basic physical properties of the materials that control their performance in solar energy conversion.



Dr Theo Hobson loading source material into a furnace. Theo's crystals have been used in the development of new designs for thin film solar cell

Highlight: Single crystal growth informs the development of thin film photovoltaics

Postdoctoral scientist Theo Hobson has been working to create single crystals of key materials in order to measure them - and hence improve their solar photovoltaic performance in devices.

In particular, Sb_2Se_3 (antimony selenide) has been of some interest since it is easy to handle and has been developing rapidly. As with other kinds of solar cells, it is deployed in a p-n junction, with the Sb_2Se_3 solar absorber being the p-type partner. Indeed it is so normal in solar cells for the absorber to be p-type that very few labs have checked whether it really is. Indeed, the conventional methods of Hall and hot probe measurement don't work easily on polycrystalline thin films. Hence Dr Hobson decided to grow single crystals of Sb_2Se_3 and measure them. Using the Bridgman method of melt growth with inert gas to suppress the Se-overpressure, he was able to grow good single crystals without voids. The surprise result was that they were not p-type as assumed in the literature, but n-type. Chemical analysis showed that the commercial high purity Sb_2Se_3 material used contained chlorine which doped it n-type. This discovery triggered two studies: The first was for us to make intentional n^+-n PV junctions using n^+-TiO_2/n-Sb_2Se_3 — these achieved over 7% efficiency, which is unequalled for a device of this kind. The second was to open up a new project on intentional p-type doping of Sb_2Se_3 with tin, which is ongoing.

The Sb_2Se_3 crystal growth also led to collaboration with others in SIRE, notably research student Nicole Fleck, to determine the Raman response of the material. Since Sb_2Se_3 is orthorhombic and has highly anisotropic bonding, it was necessary to measure single crystal samples oriented on each of the three {100} planes. The resulting Raman spectra could then be correlated with theoretical spectra in order to assign the vibrational modes.

Dr Hobson has also been active in the CZTS (Cu_2ZnSnS_4) materials system, in particular working on single crystals of the its solid solution with the selenide which is known to give the highest solar performance. Single crystals were used to generate robust compositionally dependent lattice parameter and Raman signature data. Dr Hobson was awarded his PhD in March 2020 and is now working with Ken on a project to explore new designs for thin film solar cells using n-type CdTe absorbers.

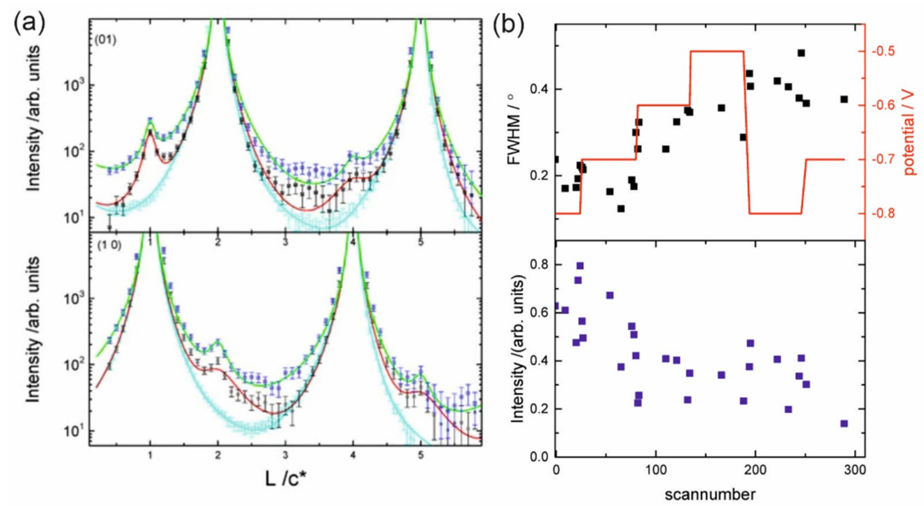
Atomic structure and charge distribution at the electrochemical interface

Yvonne Gründer

Coupling electrochemical CO_2 reduction with a renewable energy source to create high value fuels and chemicals is a promising strategy to help achieve a sustainable global energy economy. In order to develop a fundamental understanding of electrocatalytic reactions and the corresponding structure-reactivity relationships, it is necessary to apply structural characterisation techniques that can determine atomic structure at the electrochemical interface in-situ, i.e. under reactive conditions. In-situ X-ray methods have helped to develop an understanding of the underlying atomic and molecular processes associated with electrochemical energy processes.

Highlight: Structure and stability of Cu surfaces for CO_2 reduction

Copper and copper oxide electrode surfaces are suitable for the electrochemical reduction of CO_2 and produce a range of products, with the product selectivity being strongly influenced by the surface structure of the copper electrode. In our work we found that the underlying mechanism of the phosphate adsorption and deprotonation of the (di)-hydrogen phosphate is accompanied by a roughening of the copper surface. A change in morphology of the copper surface induced by a roughening process caused by the formation of a mixed copper–oxygen layer could also be observed. The stability of the Cu(111) surface and the change of morphology upon potential cycling strongly depends on the preparation method and history of the electrode. The presence of copper islands on the surface of the electrode leads to irreversible changes in surface morphology via a 3D Cu growth mechanism. The underlying mechanism of the phosphate adsorption and deprotonation of the (di)-hydrogen phosphate was accompanied by a roughening of the Cu surface. The roughening of the Cu surface through the formation of a mixed copper–oxygen layer, where the oxygen from an adsorbed phosphate species was incorporated into the surface Cu layer, is shown. The presence of Cu islands on the Cu surface leads to a 3D nucleation and growth mechanism which causes irreversible changes in surface morphology. The results demonstrate the importance of controlling the surface preparation of catalysts, as this determines the stability of the catalyst under operation conditions for the electrochemical CO_2 reduction reaction. The incorporation of oxygen into the metal surface from the adsorbed phosphate anion is a process that could also be relevant to the study of similar oxoanions, such as sulphate, and their role in the stability of electrocatalysts during oxidation processes.



Surface X-ray diffraction (A) showing the potential induced formation of twinned copper islands and (b) the subsequently occurring irreversible changes in surface morphology. Published under a Creative Commons Attribution (CC BY) license in Y. Grunder et al., Surfaces 2019, 2 (1), 145-158;

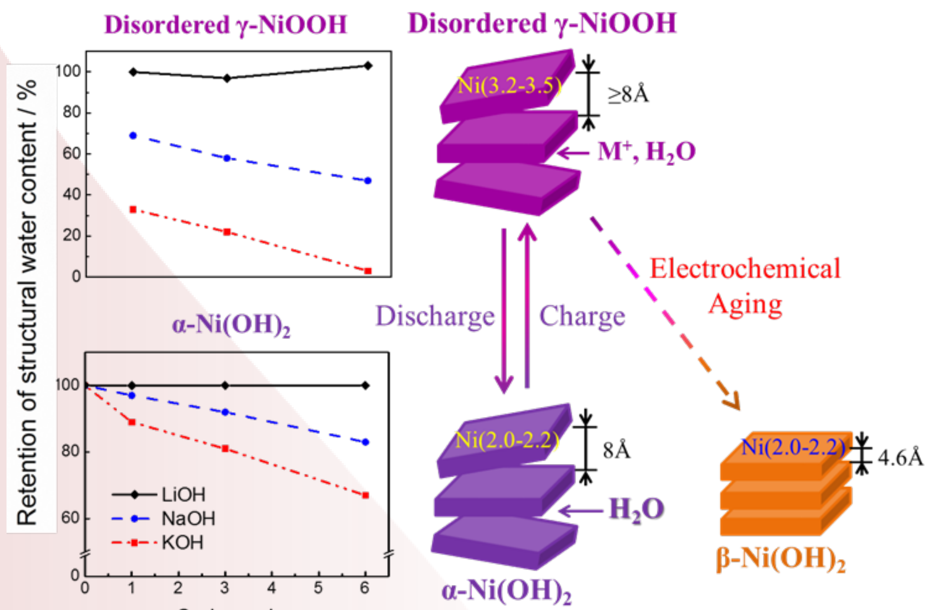
Quantifying water loss and degradation in α-$Ni(OH)_2(H_2O)$

Laurence Hardwick

Nickel hydroxide ($Ni(OH)_2$) is a key material in a variety of electrochemical applications, including nickel-based batteries, electrochemical capacitors, electrochromic devices, and electrocatalysts. However, the mechanism of how $Ni(OH)_2$ ages has not yet been fully understood. Therefore we investigated the changes in stoichiometry, and ensuing degradation for α-$Ni(OH)_2(H_2O)$ during electrochemical cycling in different LiOH, NaOH, and KOH electrolytes using a new approach combining *in situ* Raman and Density Functional Theory energy-assisted interpretation of Electrochemical Quartz Crystal Microbalance measurements. Quantitative resolution of the stoichiometric changes of the electroactive material during cycling enabled identification of a mechanism leading to the displacement of structural water and protons from the layered host upon electrochemical intercalation of the electrolyte cation.

Highlight: Atomistic understanding of phase transformations of α-$Ni(OH)_2(H_2O)$, enabling improved solutions for stabilisation

The capability to simultaneously measure changes of mass and charge of electro-active materials during a redox process makes Electrochemical Quartz Crystal Microbalance (EQCM) a powerful technique to monitor stoichiometric changes during reversible electrochemical processes. In principle, quantitative resolution of the stoichiometry of the electro-active sample during electrochemical cycling can be obtained by solving the system of equations for the EQCM mass and charge balance. Such a system of equations couples the measured changes in mass and charge through the stoichiometry of the redox process. Unfortunately, whenever more than two chemically inequivalent species are involved in the redox process, the system of equations is mathematically undetermined, having more variables (stoichiometric coefficients) than equations. In these cases, current best practice is the arbitrary reduction of the number of variables in the mass and charge balance equation, using chemical intuition to set some of the stoichiometric coefficients to fixed values. For layered ion-intercalation host materials, widespread practical approximations are the use of arbitrarily defined solvation numbers for the intercalating ions or the neglect of ion-induced displacement of structural solvent inside the host. In T-H. Wu et al., ACS Appl. Energy Mater. 3, 3347–3357 (2020), we propose an alternative approach based on the use of Density Functional Theory (DFT) to sample and screen, on an energy basis, the whole unreduced spectrum of stoichiometric coefficients compatible with EQCM measurements, leading to DFT energy-assisted resolution of stoichiometric changes during cycling. Therein we illustrate the approach by taking nickel hydroxide $Ni(OH)_2$ as an archetypal system and studying its ion intercalation-driven phase transformations in the presence of different LiOH, NaOH, and KOH electrolytes. Quantitative resolution of $Ni(OH)_2$ stoichiometry during electrochemical cycling unambiguously reveals ion intercalation to displace structural water from the layered host, promoting electrochemical degradation and ageing of the material. The process is found to be strongly dependent on the size of the electrolyte cation, with larger cations displacing larger amounts of structural water and resulting in faster degradation rates.



*Schematic on the left showing how retention rate of structural water is impacted by choice of electrolyte metal ion, which leads to a disordered γ-Ni$(OH)_2$ phase obtained from the oxidation of α-$Ni(OH)_2$ (as shown on the right). Numbers in parenthesis indicate the average oxidation state for nickel. Published under a Creative Commons Attribution License in T.-H. Wu et al., ACS Appl. Energy Mater. **3**, 3347–3357 (2020).*

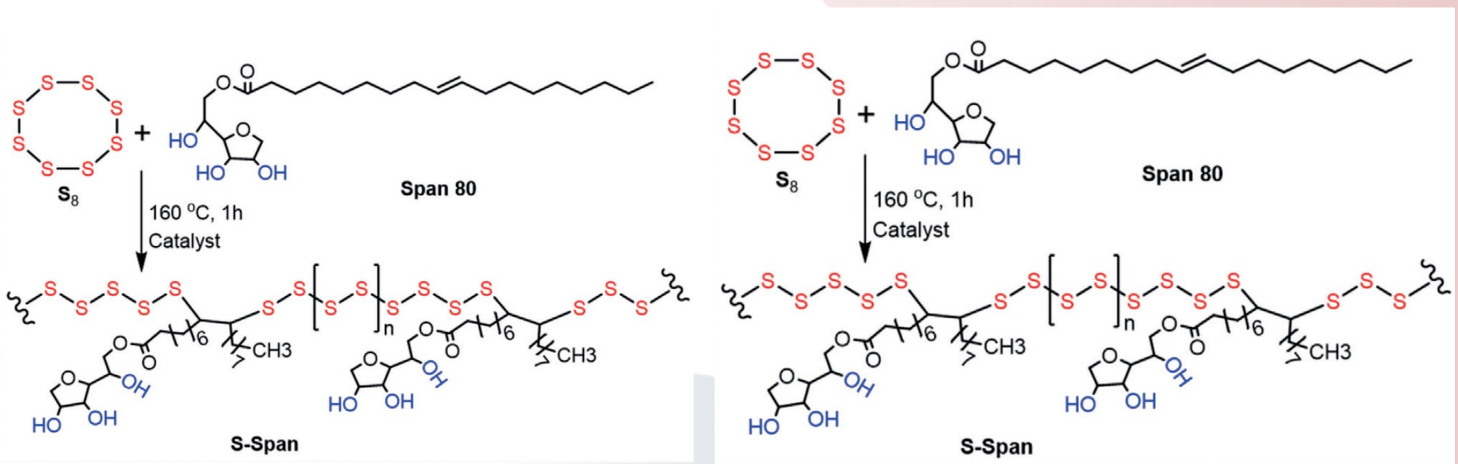
Useful materials from waste sulfur

Tom Hasell

Elemental sulfur is a waste by-product of the petrochemicals industry. It is produced in much larger quantities than it is used – leading to storage problems and vast stockpiles of sulfur being generated at oil refineries. Our group has been researching ways to turn this waste sulfur into useful materials with interesting properties. It can be turned into a polymer. Most polymers (plastics) are made from the limited petrochemical resources themselves – so making polymers instead from a by-product is more sustainable. Sulfur polymers also have some really interesting and unique properties that make them easier to recycle, and give them applications in heavy metal recovery, energy storage, infra-red transparent lenses, and antimicrobial materials. This year we congratulate the first two PhD students graduating from the group, Doug Parker and Jess Smith, as well as welcoming three new members, Veronica Hanna, Diana Cai, and Joe Dale. Dr Hasell was awarded the RSC Macrogroup UK Young Researcher Award 2021.

Highlight: Resonant transition metal donors for high mobility transparent conductors

Most polymers are made from limited petrochemical resources, and many are difficult or impossible to recycle. There are a growing number of researchers looking at how we can make plastics instead out of elemental sulfur – a largely unwanted by-product of the petrochemicals industry. Its clearly attractive to use the waste material rather than the limited resource, but also because sulfur polymers are potentially easier to recycle. But unfortunately polymers made from sulfur tend to be quite weak, which limits their applications. Peiyao Yan, the PhD student who led this work, has shown that the strength of these polymers can be increased many times over by incorporating a second type of chemical, urethane, crosslinking as well as the sulfur-sulfur bonds. What's really interesting about her work, is that the polymers she has made have shape-memory effects – they can be set in one shape, before being temporarily deformed into another. When heated a little, they will 'remember' the previous shape and go back to it. This setting process and temporary deformation can be repeated multiple times. This is a first for sulfur polymers, and despite these unusual properties, the sulfur bonds of the polymers mean they are still easy to recycle.



*Schematic representations of designed inverse vulcanisation of a pre-polymer (left) and a crosslinked polymer (right). Published under a Creative Commons Attribution License in P. Yan et al., Angewandte Chemie International Edition, **59**, 13371-13378 (2020).*

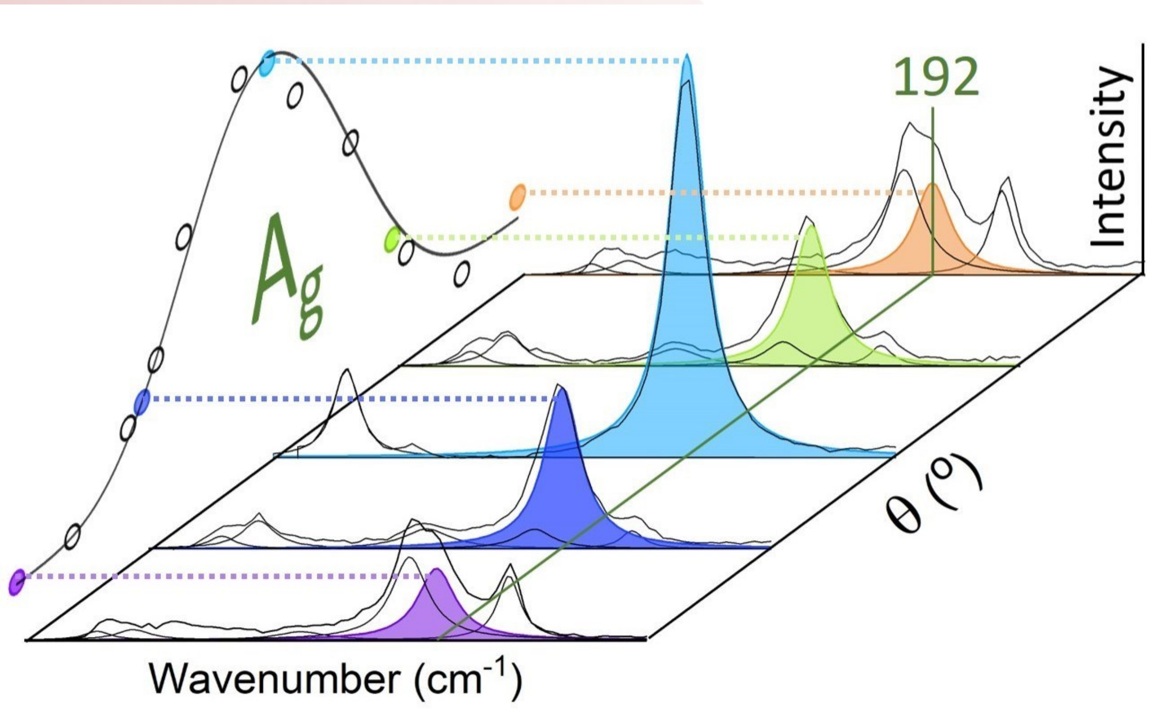
Hybrid nanomaterials: nanoplasmonics and nanophotonics

Frank Jaeckel

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: Angle-resolved polarised Raman spectroscopy of antimony selenide

Antimony selenide is a promising earth-abundant and non-toxic material for use as absorber in solar cells. While recent studies using this material have shown rapid improvements of solar cell efficiencies toward the 10% mark the fundamental understanding of this absorber is surprisingly slow to develop in comparison. In this study we investigated the vibrational properties of antimony selenide using angle-resolved polarised Raman spectroscopy. Using well defined crystallographic surfaces enabled us to reliably assign the symmetry of vibrational modes for the first time. Our results also propose a method to easily identify the desirable (001) orientation of the antimony selenide films in which solar cell performance is optimised by minimising the peak intensity of the 155 cm^{-1} mode.



The symmetry of vibrational modes can be deduced from peak intensities as a function of polarisation angle in angle-resolved polarised Raman spectroscopy. Above, the 192 cm^{-1} mode is identified as having A_g symmetry. N. Fleck, T. Hobson et al., J. Mater. Chem. A ***8****, 8337-8344 (2020).*

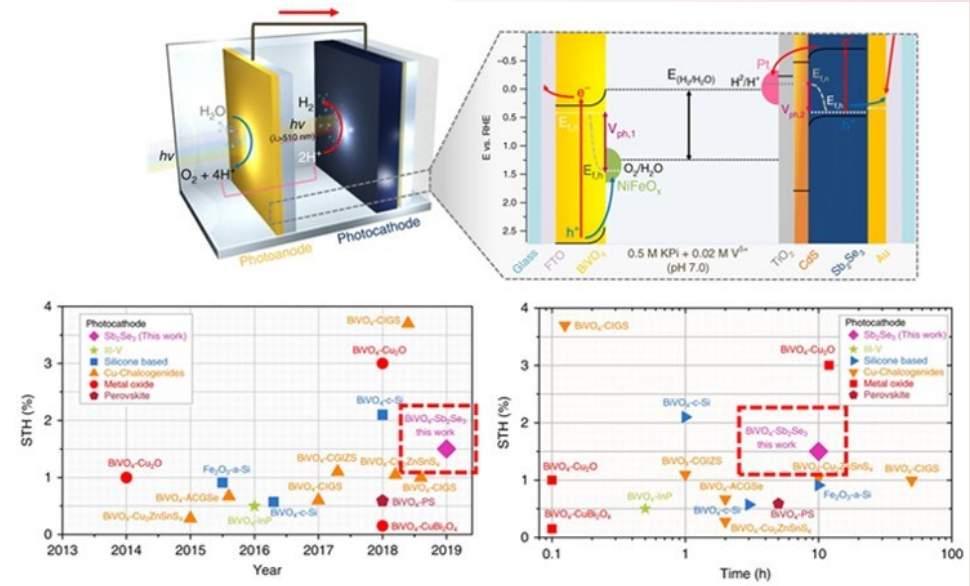
Thin film solar cell device development

Jon Major

Solar cells have the potential to generate power from a range of applications. Beyond the standard implementation as photovoltaic modules, solar cells can be integrated into buildings, vehicles, indoor devices or even used the basis for water splitting or CO_2 reduction. Each of these uses requires different considerations for the base property of the material and design of the cell structure. Our research focusses on the design, optimisation and device level physics of novel thin film solar cells, with particular focus on innovative processing techniques to improve efficiency and reduce cost.

Highlight: Sb_2Se_3 solar absorbers redesigned as solar photocathodes for water splitting.

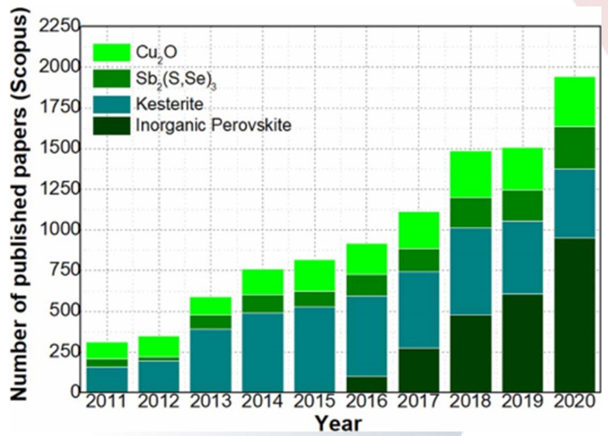
Our ongoing collaboration between SIRE and Yonsei University exploring the use of Sb_2Se_3 solar cell materials as photocathodes for water splitting led to two key publications in 2020. In work published in Nature Communications, Sb_2Se_3 was shown to be highly efficient for hydrogen production when paired with $BiVO_4$ in a "4D" tandem device. Subsequent work published in Energy and Environmental Science partnered Sb_2Se_3 photocathodes fabricated in Liverpool with wide bandgap perovskite solar cells. This led to photovoltaic– photoelectrochemical (PV-PEC) tandem devices which were able to generate hydrogen at an efficiency exceeding 10% under illumination the highest efficiency reported. W.Yang *et al*, Energy & Environmental Science, 13, 4362 (2020).



(Top) Schematic of the $NiFeO_x$/H,Mo:$BiVO_4$/FTO–Pt/TiO_2/CdS/Sb_2Se_3/Au/FTO "4D" tandem cell use for unassisted solar water splitting. (Bottom) Comparison solar-to-hydrogen (STH) efficiencies reported for various technologies in recent years

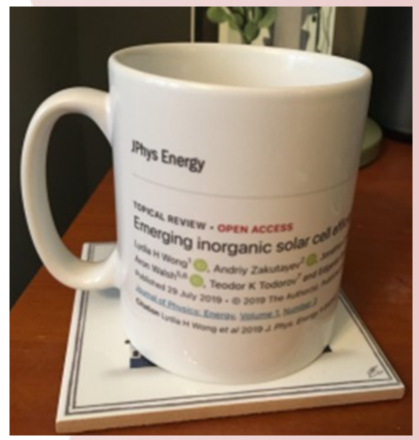
Version 2 of Emerging inorganic solar cell efficiency tables published.

The second edition of tables designed to track the development of novel solar cell technologies. The publication is a global collaboration between PV specialists and design to provide a resource for researchers to identify materials of high potential. A. Zakutayev *et al*, Journal of Physics Energy, 3, 032003 (2021).



Number of published papers in the last 10 years on emerging photovoltaics.

Even Immortalised in mug form by the editorial team at JPhys Energy



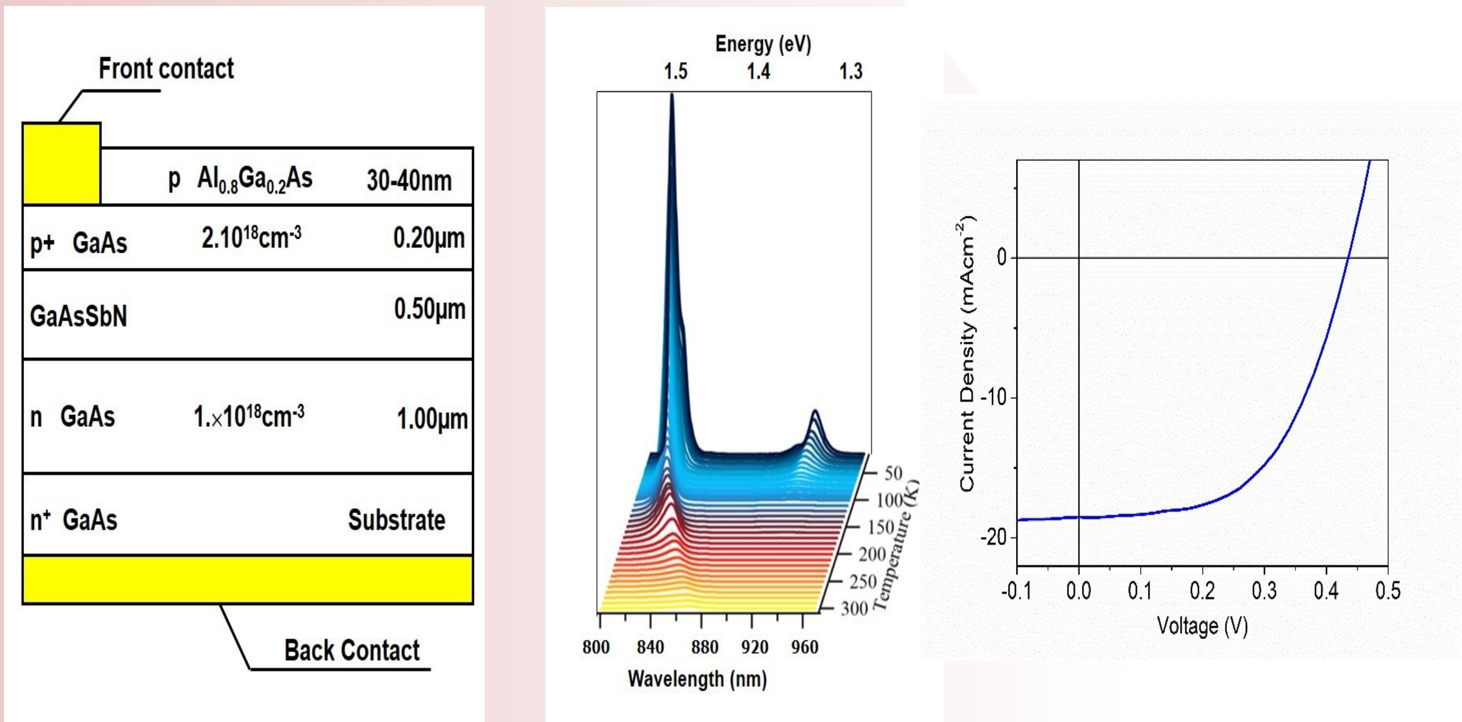
Semiconductor devices for renewable energy

Asim Mumtaz

I am a member of the solar energy materials and solar cells group. My interests are in semiconductor devices, particularly solar cells and power semiconductor devices. In terms of solar cells, I have been involved in projects relating to tandem solar cells, which have included crystalline III-V semiconductors and perovskite solar cells. I also have an interest in modelling and fabrication of high-performance power devices employing wide band gap semiconductors such as silicon carbide and gallium nitride. Such power devices are essential for energy conversion applications — for example inverters used in renewable energy systems. I have also undertaken a project on electrodes for lithium ion cells driving towards improved energy capacity and durability.

Highlight: Liquid phase epitaxy of III-V multi-junction solar cells

Multi-junction solar cells, according to the detailed balance limit, should be able to achieve power conversion efficiencies of over 50%. Work on new materials for multi-junction solar cells is necessary for improvements beyond the current state of the art. We evaluated the use of GaAsSbN, which has shown promise for multi-junction solar cells. Epitaxial growth of this material in this work was been achieved via liquid phase epitaxy, as it can produce high quality crystalline layers. GaAsSbN has the advantage of being a dilute nitride and its band gap can be controlled effectively through adjusting the proportion of antimony (Sb) and nitrogen (N) to GaAs. Also, variations in the Sb content affects the valence band offset while the nitrogen content primarily affects the conduction band offset. This makes it possible to tune the conduction and valence band offsets independently, while keeping the lattice matching to GaAs. This work was completed in collaboration with colleagues at the Central Laboratory of Applied Physics, Bulgarian Academy of Sciences. Complete GaAsSbN p-i-n solar cells were developed and tested.



*(left) Schematic structure of single-junction p-i-n solar cells based on compensated GaAsSbN heterostructure grown by LPE (centre) Temperature dependent PL spectra of solar cell structure in the range 15-300K. (right) a current –voltage curve of a GaAsSbN p-i-n solar cell. Malina Milanova et al, Single-junction solar cells based on p-i-n GaAsSbN heterostructures grown by liquid phase epitaxy, Solar Energy, **208** 2020 659*

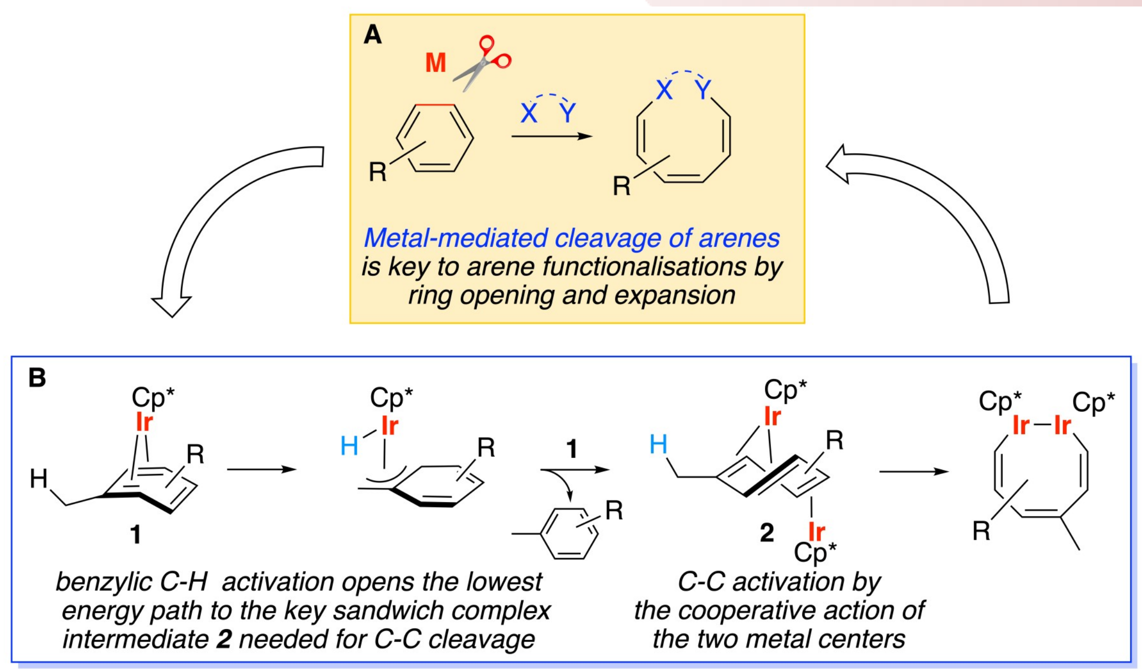
Homogeneous catalysis and organometallic chemistry

Alexey G. Sergeev

We focus on improving existing catalytic reactions and discovering new ones for the synthesis of value-added chemicals and fuels from hydrocarbon natural resources at mild temperatures and with minimum side products. In particular, 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 by well-defined soluble metal complexes. The goal is to identify key principles enabling the high selectivity and activity in these fundamental steps and translate these findings into synthetically useful catalytic reactions for making functionalised molecules with a broad range of applications. To achieve this goal, we study both mechanisms and synthetic applications 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: Selective cleavage of un-activated arene ring C-C bonds by iridium: Key roles of benzylic C-H activation and metal-metal cooperativity

The cleavage of aromatic C-C bonds is central for the conversion of petroleum and coal into a range of industrial chemicals ranging from fuel to pharmaceuticals. However, the progress in designing mild, clean and safe methods for such conversion is hampered by the lack of experimental examples of selective oxidative addition of aromatic C-C bonds and poor understanding of the factors that favour insertion into the stronger aromatic C-C bonds rather than the weaker C-H bonds. Recently, we reported the uniquely selective insertion of a transition metal into C-C bonds in a range of industrially important arenes (*Angew. Chem Int. Ed.* **2017**, *56*, 3266; *J. Am. Chem. Soc.* **2019**, *141*, 6048). We investigated the mechanism of this insertion by experimental and computational methods and showed that this ring cleavage requires reversible scission of a benzylic C-H bond and co-operativity of two Ir centres sandwiching the arene in the product-determining intermediate. The mechanism explains the selectivity and scope of this unique aromatic C-C activation and may help to design more mild and selective methods for making value-added chemicals from aromatic hydrocarbons.



(A) Metal-catalysed functionalisation of the aromatic C-C bond; (B) The brief mechanism for the mild and selective activation of aromatic C-C bonds by Ir (I). Published under a Creative Commons Attribution License in Chem. Sci. ***12*** *2021 3568.*

Nanoencapsulation for energy storage, generation and sustainable coatings

Dmitry Shchukin

Research activities of the group include development of the composite hollow nanocontainers (capsules) for encapsulation of the energy-enriched materials, food components, drugs, biocides and corrosion inhibitors — and the development of nanocontainer-based active coatings for thermo-regulating, self-healing and antifouling applications.

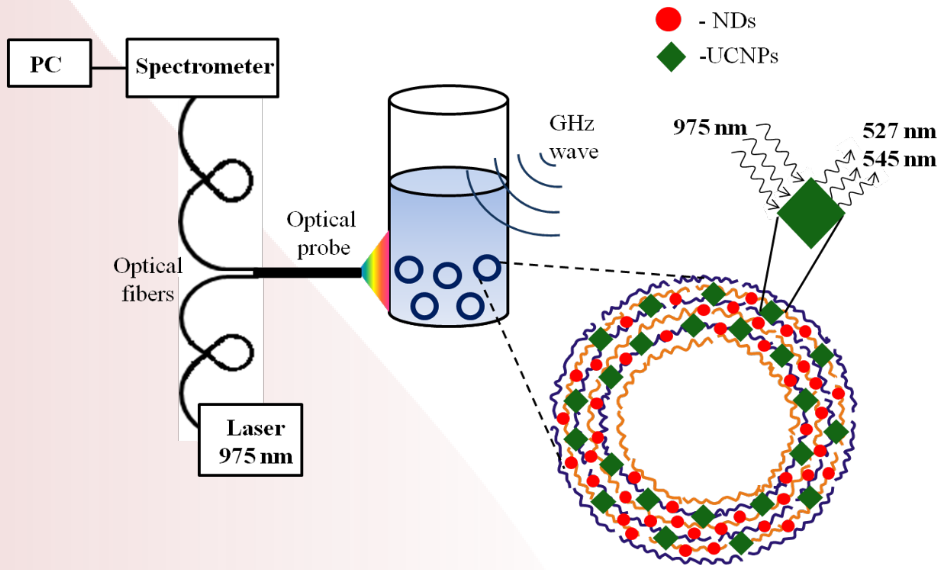
Particular attention in 2020/21 has been paid to high-throughput methods of the synthesis of active capsules using robotic and AI technology platform.

Another research direction is synthesis of nanomaterials at the ultrasonic cavitation interface to replace high temperature chemical processes. The group has joint research projects/laboratories with China (NPU Xi'An, CAS Beijing), Russia (ITMO and Gubkin Universities) and USA (Louisiana Tech University-*Latech* and Georgia State University) resulting in exchange of staff between collaborators.

Highlight: Measurements of the local temperature on nanoscale level

The multilayer structure of the capsules was designed to create a polyfunctional system intercalating with nanodiamonds (NDs) and upconversion nanoparticles (UCNPs) into the polyelectrolyte shell. NDs empower local overheating to the microcapsules, while UCNPs provide opportunity to luminescent thermal sensing. The capsule membrane was formed by sequential deposition of the oppositely charged macromolecules on the surface of the colloidal particles

The sensitizer effectively absorbs NIR-photon and transfers from the ground to excited metastable state followed by non-radiative resonance energy transfer between sensitizer coupled with an activator. The activator normally possesses ladder-like arranged energy levels that promote energy accumulation from upconversion by the photon absorption. Microwave triggering followed by the capsule heating results in the controlled destruction of the polyelectrolyte shell with subsequent cargo release. UCNPs luminescence was utilized to determine the local temperature of the capsule shell at nanoscale under GHz treatment.



Schematic illustration of local temperature measurements inside capsule nanoshell based on UCNP photoluminescence. NDs – nanodiamonds, UCNPs—upconversion $NaYF_4$ nanoparticles doped with pairs of trivalent lanthanide ions, which play roles of sensitizer (Yb^{3+}) and activator (Er^{3+}). Published under a Creative Commons Attribution License in T. Borodina et al., Polymer ***212****, 123299 (2021).*

The mutual entrapment of NDs and UCNPs allows one to control the information concerning thermal effects inside the capsule and in the shell. As a result, homogeneous heating of the polyelectrolyte layers surrounding NDs opened the capsule shell. The developed multifunctional capsules allow one to monitor and control temperature exchange between nanoconfined phase change materials in 3D directions. The use of the upconversion nanoparticles either in planar nanolayers or in capsules shell is more effective than other known methods for measuring heat exchange between nanomaterials in real time. Moreover, the nanoscale precision makes possible to detect the effect of the size reduction of the phase change materials on their heat storage and heat transfer properties.

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PhD Graduates in 2020/21

Dr Tom Baines
Optimisation of $CdTe_{(1-x)}Se_X$ and
$Mg_XZn_{(1-x)}O$ layers for CdTe PV
devices
Supervisors: Jon Major,
Ken Durose

Dr Daniel Cheung
The potential of the ultrasonic cavita-
tion phenomenon for the synthesis and
modification of novel semiconductor
heterojunction photocatalyst for photo-
catalytic water splitting and dye
degradation
Supervisors: Dmitry Shchukin,
Alex Cowan

Dr Tom Featherstone
Novel dopants in TCOs for im-
proved infra-red transparency
Supervisors: Tim Veal, J
on Major, Ken Durose

Dr Claudia Gatti
Iridium-mediated C-H function-
alisation under mild conditions
Supervisors: Alexey Sergeev,
Dmitry Shchukin

Dr Theodore Hobson
Growth and properties of
bulk CZTSSe and Sb_2Se_3
for solar cells
Supervisors: Ken Durose,
Jon Major

Dr Sophie Hodgkiss
Developing rapid powder dif-
fraction analysis for efficient
characterisation of new
materials
Supervisors Tony Lopez-
Sanchez

Dr Ashlea Hughes
Probing structure and dynamics
in advanced molecular materi-
als by solid state nuclear mag-
netic resonance
Supervisor: Frederic Blanc

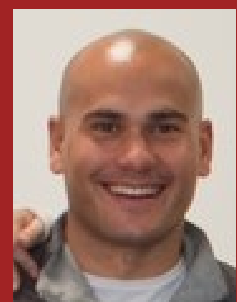
Dr Javier Eduardo Pérez Mejía
Catalytic conversion of cellulose
and cellobiose into glucose, sorbitol,
gluconic acid and glucaric acid over
carbon-based catalysts in batch and
continuous microwave reactors
Supervisor: Tony Lopez-Sanchez

Dr Philip Murgatroyd

Experimental theoretical studies
of correlated electron systems

Supervisors: Jon Alaria, Tim Veal

Dr Graeme O'Dowd
FeS_2 thin film photoelectrodes from
nanostructured colloidal precursors
Supervisors: Frank Jäckel , Yvonne
Gründer



Dr Romen Padilla
Morphology Control in Colloidal
Metal Nanoparticle Synthesis and
their Application to Catalysis
Supervisor: Tony Lopez-Sanchez

Dr Douglas Parker
Inverse vulcanised sulfur polymers
for heavy metal remediation
Supervisor: Tom Hasell

PhD Graduates cont….

Dr Robyn Presland
The preparation and catalytic ring opening diborylation of 1-substituted biphenylenes
Supervisor: Alexey Sergeev

Dr Samuel Petcher
Thiopolymers: Applications in water remediation and development
Supervisor: Tom Hasell

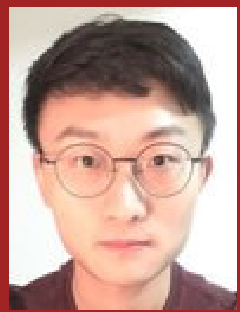
Dr Jack Swallow
Physics of existing and novel transparent conducting oxide semiconductors
Supervisors: Tim Veal, Vin Dhanak

Dr Siti Nurbaya Supardan
Study of high-k dielectrics and their interfaces on semiconductors for device applications
Supervisor: Vin Dhanak

Dr Verity Piercy
Photocatalytic materials for the reduction of CO_2 to fuels
Supervisor:
Alex Cowan

Dr Tom Shalvey
Interface modifications and doping approaches for CdTe thin film solar cells
Supervisors: Jon Major, Ken Durose

Dr Dong Xiao
Carbocations in heterogeneous catalysis caught in the act by DNP enhanced multidimensional and multinuclear NMR
Supervisor: Frederic Blanc



Dr Ruowei Yi
Dual-functional graphene/ $Ti_3C_2T_x$-based Interlayers towards high-performance Li-S batteries
Supervisor: Laurence Hardwick

Dr Huw Shiel
Band alignments and interfaces in antimony selenide solar cells
Supervisors: Jon Major,Tim Veal, Vin Dhanak

Dr Jessica Smith
Inverse vulcanisation of elemental sulfur for functional materials
Supervisor: Tom Hasell

Dr Xiaolei Zhu
Fabrication of nanocomposite phase change materials by encapsulation and form-stabled compound and study of their properties
Supervisor: Dmitry Shchukin

Research Grants Held

A total of > £30m is currently held by SIRE investigators. New grants in 2020/21 are highlighted with an asterisk.*

Engineering & Physical Sciences Research Council

T Hasell Bridging the TRL gap to enable commercialisation of sorbent for mercury capture and precious metal recovery*	£39,983
T McDonald & **D Shchukin** Active mapping of biological substrates for crop care and personal care applications*	£45,924
A Cooper & **A Cowan** Autonomous mobile robot chemists*	£902,085
A Vezzoli Quantum-enhanced molecular piezoresistivity*	£387,114
J Xiao & **J Lopez-Sanchez** Iron-catalysed oxygenation with O_2	£349,348
F Blanc Very-high field NMR in the physical and life sciences at the university of Liverpool	£2,000,000
G Zoppi & **J Major** Nanoscale interfacial engineering of antimony-based absorber materials for PV applications (NECEM)*	£206,000
W Van Der Hoek & **A Cowan** EPSRC Capital Award emphasising support for ECRS	£336,301
J Lopez-Sanchez Impact acceleration account - University of Liverpool 2017	£27,211
T Hasell Li-S polymers for stable and long-life Li-S batteries*	£14,069
F Blanc Connect NMR UK: A national NMR network for the physical and life sciences	£382,000
C A Lucas & **Y Grunder** Xmas: The UK materials science facility at the ESRF	£3,515,607
M Rosseinsky & **J Alaria** Chemical control of function beyond the unit cell for new electroceramic materials	£928,,091
P Weightman & **V Dhanak** FLUENCE: Felix Light for the UK: Exploiting novel characteristics and expertise	£507,705
J Major Capacitance spectroscopy led process innovations to improve Voc in CdTe thin film solar cells	£810,102
K Durose, A Walker EPSRC centre for doctoral training in new and sustainable PV	£5,326,776
W van der Hoek, I Sandall, **F Jaekel**, L O'Brien & **A Vezzoli** EPSRC Core equipment award 2020*	£594,430
K Durose & **J Major** New designs for thin film solar cells*	£509,722
M Rosseinsky & **A Cowan** Flexible routes to liquid fuels from CO_2 by advanced catalysis and engineering	£987,874
M Rosseinsky & **J Alaria** Digital navigation of chemical space for function*	£8,699,373
A Cowan Application of electrocatalysts under industrially relevant conditions: testing the feasibility of converting carbon dioxide produced during bioethanol conversion – working at higher current densities*	£33,202
A Cowan Spectroscopy-driven design of an efficient photocatalyst for carbon dioxide reduction	£903,680
A Cowan REDEEM-electrocat: Rethinking electrode design – emergent electronic and magnetic effects in electrocatalysis*	£127,498
K Badcock, **A Cowan**, **F Jaeckel**, **J Major** & J L Walsh EPSRC capital award emphasising support for ECRS	£225,000
F Blanc The UK High-field solid-state NMR national research facility at Warwick*	£2,650,000
W Van Der Hoek & **F Jaekel** EPSRC capital award emphasising support for ECRS	£225,000
M Rosseinsky & **J Alaria** Correlated metals as transparent conductive coatings	£24,877

European Commission

L Hardwick BIGMAP (Battery Interface Genome – Materials Acceleration Platform) H 2020	£554,000

European Research Council

D Shchukin New shell components for encapsulation of crystallohydrates	£1,594,670

The Faraday Institution

L Hardwick, M Rosseinsky CAT-MAT: Li-ion cathodes*	£590,101
N Browning, **A Cowan & L Hardwick** Quantitative imaging of multi-scale dynamic phenomena at electrochemical interfaces	£410,078
L Hardwick SOLBAT - The solid-state (Li or Na) metal-anode battery	£217,557
F Blanc Realising the potential of NMR to probe Li conduction pathways	£2,000
L Hardwick Faraday Challenge: Towards a comprehensive understanding of degradation processes in EV batteries*	£234,069
L Hardwick SOLBAT—The solid state (Li or Na) metal anode battery (extension)	£38,567

Henry Royce Institute

A Cowan & **L Hardwick** Materials for end-to-end hydrogen application*	£326,026

Industrial

Croda (UK), T McDonald & **D Shchukin** Active mapping of biological substrates for crop care and personal care applications*	£10,000
Bristol-Myers Squibb Pharmaceuticals LTD (UK), **F Blanc** DTP studentship - industry top-up	£80,000
Pilkington Group Limited (UK), **T Veal**, **V Dhanak** & **J Major** Studentship - industry top-up	£10,000
Johnson Matthey PLC (UK), **L Hardwick** Using SHINERS technology to solve challenging interfacial problems in catalytic and battery applications*	£58,860
Semefab Ltd, **A Mumtaz** Novel devices using wide band gap semiconductors*	£5,000
Lubrizol, **L Hardwick** Ionic Liquid and redox mediator electrolyte blends for long-life lithium-air batteries	£90,000

Innovate UK

L Hardwick G-Cap supercapacitor in all-terrain vehicles	£223,801

Leverhulme Trust

A Sergeev Arene functionalizations through metal-mediated scission of aromatic rings	£288,039
A Cowan Gel-based photoelectrodes for clean fuels	£125,987
F Blanc Dynamic nuclear polarisation from paramagnetic metal ions*	£263,000

NATO (Belgium)

D Shchukin Functional textiles for uniforms	£59,924

Research England

A Cowan Carbon dioxide reduction using molecular catalysts to make useful products*	£33,871
A Cowan Industrial strategy HEIF allocation 2019-2020	£9,655

Royal Academy of Engineering

A Mumtaz Novel devices using wide band gap semiconductors	£38,481

Royal Society

J Alaria Advanced functional materials for waste heat harvesting and green computing, a bridge between thermoelectricity and spin-electronics	£12,000
Y Grunder Charge distribution at the electrochemical interface*	£696,372
T Hasell Carbonised sulfur polymers for gold extraction*	£92,087
A Vezzoli Molecular engineering in quantum thermoelectrics*	£16,800
T Hasell Sulfur polymers for optical and antimicrobial applications*	£685,086
A Vezzoli Single-entity electronics and photonics of chemically wired nanocrystals*	£1,149,367
D Shchukin Thermal management of perovskite solar cells based on layer-by-layer assembled liquid metal nanoparticles	£11,940
Y Grunder Elucidating the relationship of Interfacial charge distribution and structural behaviour and stability of bimetallic electrocatalysts	£38,821
T Hasell Enhancement of the mechanical properties of sulfur based polymers, and investigation of their behaviour in supercritical carbon dioxide	£238,481
J Alaria Linking the magneto-electric properties of novel multiferroic materials at the micro- and nano- scale for beyond CMOS data storage technology	£12,000

UK-India Education and Research Initiative

I Mitrovic & **V Dhanak** Dielectric engineering on GaN for sustainable energy applications	£45,592

UK Research and Innovation

A Cowan NIC3E: National interdisciplinary centre for circular chemical economy*	£853,759
A Cowan UKRI CoA: Spectroscopy-driven design of an efficient photocatalyst for carbon dioxide reduction*	£903,679
A Lyons, **T Hazell** & **F Blanc** Post-consumer resin - Understanding the quality-performance linkage for packaging*	£1,897,765


Jon Alaria


Frédéric Blanc


Alex Cowan


Vin Dhanak

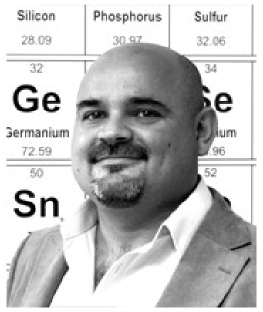

Ken Durose


Yvonne Grunder


Tom Hasell


Laurence Hardwick


Frank Jaeckel



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