UNIVERSITY OF
CAMBRIDGE

THE WINTON PROGRAMME FOR THE Physics of Sustainability

ANNUAL REPORT
2017

This is the sixth Annual Report of the Winton Programme for the Physics of Sustainability and provides information about some of the activities and research highlights that have been enabled by the £20 million donation by David Harding, an alumnus of the Physics Department.

The donation has provided the freedom to perform 'blue-skies' research into new areas that may provide the breakthroughs that are needed to ensure we do not run out of natural resources, whilst meeting our targets for limiting global temperature rise.

REVIEW

Richard Friend,
Cavendish Professor of Physics

The Winton research community brings together a broad and diverse set of research interests both within the Cavendish Laboratory and across the University. It is thriving in the Maxwell Centre which provides a very attractive working environment, both the offices and more particularly, the many informal meeting spaces. The Winton Programme has helped define the research culture in the building and I am confident that this is a place where barriers between research silos are broken down and new research ideas are generated. I think the accounts of Winton-supported research in this annual report provide the evidence for this. Though the 'people space' in the Maxwell Centre was quickly filled, bringing new equipment facilities into the laboratory space on the ground floor has been a slower process. We have worked hard to put together facilities that are both state-of-the art but that are also available to a wide user base – this will make possible the unplanned and the unexpected experiments that launch new fields. With Winton support, we are currently setting up an ultrafast transient photoluminescence confocal microscope, and jointly between the Cavendish and Engineering, a Tera-Hertz spectroscopy facility. Many of the research facilities provided for the Henry Royce Institute for Advanced Materials are now being installed in the Maxwell Centre. We expect these facilities will help Cambridge play an important role in the national Faraday Institution, launched to develop new batteries, principally for transportation.

The 2016 symposium focussed on the science that underpins solar cells; the falling cost of conventional silicon cells, driven by the huge increase in manufacturing scale, has brought solar to grid parity and below in sunnier parts of the world, and we learned at the symposium that there are exciting prospects for further performance advances enabled by new science and new technologies. Together with very rapid cost reductions in wind energy, we face the challenge that a substantial fraction of our electricity generation will be 'green' but intermittent. This year, therefore, the Winton Symposium addresses the interconnected challenges of storing electrical energy and moving it around. Batteries and fuel cells are critical for this, certainly for the electrification of transport, and as prices fall, may play a big role in grid storage. Technologies for the electricity grid are developing rapidly; high voltage electronics makes DC transmission systems possible through DC to DC voltage conversion, and superconducting electricity transmission offers the future prospect of ever lower transmission losses. In the longer term, hydrogen fusion reactors promise 'non-intermittent' electricity generation; success in this depends on meeting some very exacting materials and engineering challenges.

PROGRAMME UPDATE

Nalin Patel, Programme Manager

Overview

The Winton Programme for the Physics of Sustainability has now been established for over six years during which time it has supported six cohorts of both Winton Scholars and Winton Advanced Research Fellows. This investment in young researchers has remained a constant theme of the Programme, enabling talented ambitious people to develop their ideas in an environment that encourages interdisciplinary collaborative research. The Programme is based in the Physics Department, with the majority of activities now taking place in the Maxwell Centre; this move has facilitated increased interactions both within the Winton community as well as within the University and colleagues from further afield.

People

The sixth cohort of Winton Scholars is well into their research programmes (see list of Scholars and their projects). The Programme continues to attract excellent candidates from around the world, with research in a broad range of topics including joint supervision with other departments.

Three new Winton Advanced Research Fellows have been appointed, each bringing new capabilities to the Cavendish through their independent research. Dr Chiara Ciccarelli is setting up a THz spectroscopy system to study spin effects in magnetically ordered materials. Dr Felix Deschler will explore electronic states in hybrid materials systems with high temporal and spatial resolution. Dr Alpha Lee will work on statistical physics for soft matter by combining experiments and simulations with machine learning. Further details of the Fellows and their research is provided in this report.

Two of our Fellows are also moving on to permanent research positions. Dr Andrew Morris, who has been working on materials discovery, has secured a senior Birmingham fellowship at the University of Birmingham. Dr Alex Chin, who has being developing the theoretical aspects of the emerging field of Quantum Effects in Bio-Organic Nanotechnologies, will join the *Centre national de la recherche scientifique* (CNRS) in France, creating a new Theory Group within the *l'Institut des NanoSciences de Paris* (*l'université Pierre et Marie Curie*, Paris). Both will continue to interact with the Programme and co-supervise students and projects with collaborators in Cambridge.

The Winton International Advisory Board, which provides strategic advice on the direction of the Programme, welcomes two new members. Professor Albert Polman, who leads the Photonic Materials Group at FOM Institute for Atomics and Molecular Physics (AMOLF), Netherlands and Professor Laura Diaz Anadon who holds the Professorship of Climate Change Policy at the University of Cambridge.

Connections

With the majority of the Winton activities now housed in the Maxwell Centre, there are increased opportunities for 'chance encounters' between the Winton community and others who are working in or passing through the building. This has been boosted by EPSRC funding received for a networking programme CAM-IES (Centre for Advanced Materials for Integrated Energy Systems) and the new open-access facilities funded by the Henry Royce Institute for Advanced Materials, both of which are operated through the Maxwell Centre and have strong links with the Winton Programme.

Other new connections are being enabled by the Winton Berkeley Exchange Programme. This facilitates interactions between the Winton Programme and the Kavli Energy NanoScience Institute (Kavli ENSI) at the University of California, Berkeley including research activities that are related to the two Programmes from across both universities. The aim is to develop complementary research between

the two Programmes with funding available for exchanges in both directions for PhD students, postdoctoral researchers and faculty members for sabbatical visits.

The first exchanges have taken place, and further exchanges are planned for the coming year. Dr Luis Pazos-Outón from the optoelectronics group in Cambridge visited Professor Eli Yablonovitch's group located in the UC Berkeley college of Engineering. During his four-month visit, he worked on a project to develop thermal photovoltaic devices, which uses a hot source of black body radiation surrounded by photovoltaic cells that can lead to very high efficiency conversion of radiation to electrical power. Luis has subsequently been awarded a Heising-Simons Postdoctoral Fellowship at the Kavli ENSI which will enable him to continue the thermo-voltaic device work and the related project on developing a thermo-photonic bottle for vaccine delivery.

Lissa Eyre is a PhD student in Cambridge, jointly supervised by Dr Hannah Joyce in Engineering and Dr Felix Deschler in Physics. During her exchange she worked in Professor Jim Schuck's nano-optical imaging group at the Lawrence Berkeley National Laboratory for 3-months. During this time she set up a time-resolved anti-Stokes Raman experiment with high spatial resolution, which can be used to study the photo-physics of metal-halide perovskite nanostructures, which are being extensively developed for next generation solar cells.

A one-week Exchange Programme workshop was held this year with four days at an off-site venue followed by two days at the UC Berkeley campus. The workshop involved around 30 researchers related to the Kavli ENSI and a similar number from the Winton Programme and the EPSRC Centre for Doctoral Training in Nanoscience and Nanotechnology. Participants exchanged ideas about their research areas and then formed groups with the aim to generate ideas that would form the basis of a grant proposal. A number of faculty members, led by Professor Jeremy Baumberg from Cambridge and Professor Eli Yablonovitch from UC Berkeley, attended the workshop providing advice and mentoring to the attendees as well as judging the written proposals and presentations.

Above: Attendees of the Winton-Berkeley Exchange Programme workshop.

WINTON SCHOLARS ARRIVING IN 2016/17

Antonis Alvertis
Supervisors: Dr Alex Chin and Dr Akshay Rao
Optoelectronics Group and Theory of Condensed Matter Group
"Modelling of electronic structure and ultra-fast quantum dynamics in excited organic semiconductors"

Zahra Andaji-Garmaroudi
Supervisors: Professor Richard Friend and Dr Sam Stranks
Optoelectronics Group
"Perovskite structure nanocrystals for light harvesting and light emission"

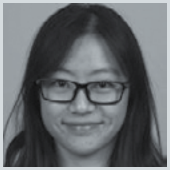
Virgil Andrei
Supervisor: Professor Erwin Reisner
Department of Chemistry
"Hybrid devices for water splitting"

Hope Bretscher
Supervisor: Dr Akshay Rao
Optoelectronics Group
"Ultrafast spectroscopy to improve solar cells"

Sivapalan Chelvaniththilan
Supervisor: Dr Rosanna Collepardo-Guevara
Biological and Soft Systems Group
"Investigating the link between epigenomes and chromatin structure to guide the design of new sustainable nanochromatin devices"

Theresa Jakuszeit
Supervisors: Dr Ottavio Croze and Professor Alison Smith
Biological and Soft Systems Group and Department of Plant Sciences
"Physics of bacterial motility and chemotaxis in porous media for efficient bioremediation"

Raj Pandya
Supervisors: Dr Akshay Rao and Professor Ulrich Keyser
Optoelectronics Group and Biological and Soft Systems Group
"Investigating energy and charge flow in biomimetic systems using ultrafast microscopy"



Wenting Wang
Supervisors: Professor Chris Abell and Professor Jeremy Baumberg
Department of Chemistry and Nanophotonics Group
"Trace analyte detection by assembling Au nanostructures in microdroplets"

Tianheng Zhao
Supervisors: Dr Silvia Vignolini and Dr Erika Eiser
Department of Chemistry and Optoelectronics Group
"Responsive structural photonic materials for food safety sensors & indicators"




WHERE ARE THEY NOW?

A number of the Winton Scholars have now moved on from research in Cambridge to pursue a range of careers in industry or academia. Some examples are described below.

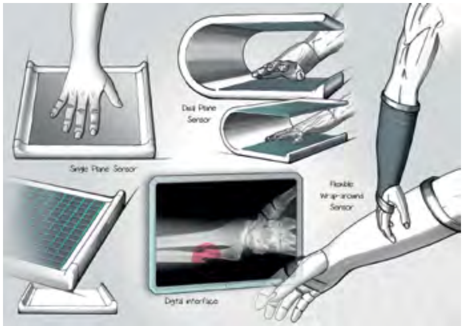
Dr Jan Mertens
(Winton Scholar 1st cohort)

Jan is working in the 'highly automated driving' project at Bosch. Automating driving is a new challenge for our society that needs to be addressed to make transportation safer, more comfortable and to contribute to a more sustainable future.

He works at the interface between research and implementation of novel sensing technologies to enable automated driving. Linking different stakeholders within Bosch, he identifies requirements addressing the complex interplay of hardware and software necessary in sensing solutions. He is constantly seeking emerging concepts to fabricate new generations of sensors, in particular optical sensors, to perceive and track the environment while driving.

Dr Sarah Morgan
(Winton Scholar 2nd cohort)

Sarah is now a Research Associate at the Cambridge Brain Mapping Unit, working with Professor Ed Bullmore to study human MRI brain images using graph theoretical approaches. In particular, her research focuses on identifying graph theoretical biomarkers to diagnose and predict disease trajectories for individuals with schizophrenia based on their MRI brain scans. This work is part of a large EU project called PSYSCAN. More generally, Sarah is interested in the range of biological problems to which complex networks can be applied, across spatial and temporal scales.



Dr Vahe Tshitoyan
(Winton Scholar 2nd cohort)

Vahe works for Zedsen, a London based company that has developed intelligent and flexible 3D sensors using advanced algorithms that will have a transformative impact on industries that include healthcare, life sciences, automotive, aerospace and security. The sensors can identify materials whether solid, liquid, or powder, measure pressure, weight, downforce and lift, and create images by scanning inside objects. The sensors are printed, making them low-cost, easy to configure, embed and scale. He is mostly involved in signal processing and machine learning research to make our sensors smarter. He also works on physics models of advanced capacitive sensors and corresponding image reconstructions algorithms.

Dr Hannah Stern
(Winton Scholar 2nd cohort)

Hannah Stern has recently completed her PhD with Professor Richard Friend in which she investigated the mechanism of endothermic singlet exciton fission. Since then, she has taken up a Junior Research Fellow at Trinity College. During her fellowship she will be exploring spectroscopic techniques for measurements on the single molecule level, in particular super resolution fluorescence imaging and spectrally-resolved single molecule experiments. This work is carried out in the groups of Professor David Klenerman and Dr Steven Lee, with collaborations with the Departments of Physics and Engineering.

Above: Schematic of Zedsen application

WINTON CONNECTIONS

Lata Sahonta, Programme Manager for Energy Materials and CAM-IES

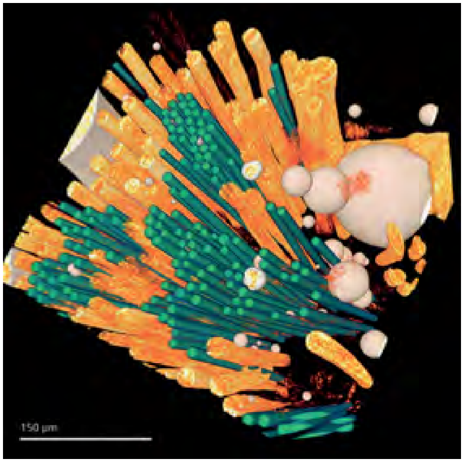
The Maxwell Centre is the perfect environment for the Winton community of Scholars and Advanced Research Fellows to engage with other researchers to develop collaborations, as well as take advantage of excellent shared research facilities. A major contribution to the Maxwell Centre facilities in 2017 has been the installation of world-class research equipment purchased through the £10 million investment awarded by the Henry Royce Institute for Advanced Materials, the UK's national materials research centre. The Cambridge Royce facilities at the Maxwell Centre will be open for use as a national facility by both academic and industrial researchers in early 2018.

Henry Royce Institute for Advanced Materials

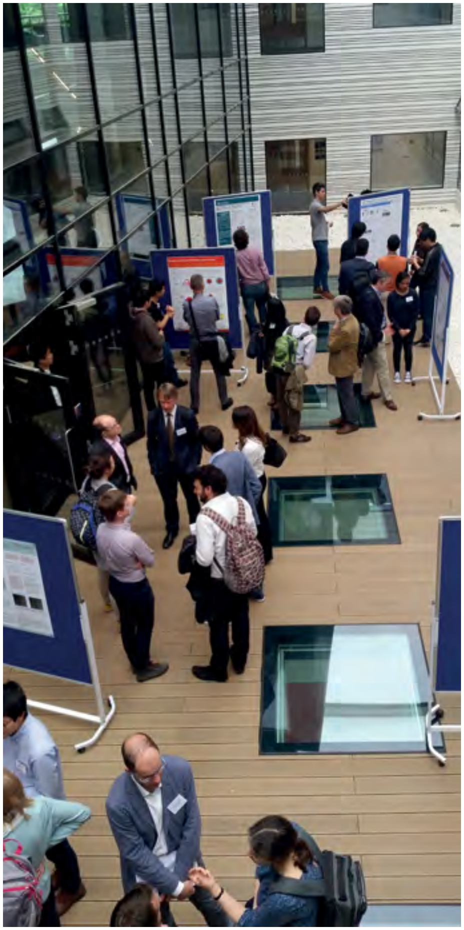
The Cambridge Royce facilities are focused on promoting research within the theme of *Materials for Energy-Efficient ICT*, to facilitate the fabrication, testing and packaging of device materials and systems with reduced consumption of resources and energy in their production and use. The Cambridge Royce equipment comprises a range of advanced materials growth and device characterisation tools for applications in efficient energy generation, energy storage, and energy use. These goals match splendidly with the research aims of the Winton Programme, and are vitally important for cutting-edge basic research and novel industrial applications in the energy sector.

Examples of Maxwell Centre equipment provided by the Henry Royce Institute include:

Cluster Tool: ten custom-built interconnected gloveboxes that integrate different deposition, metrology, thin film encapsulation, and packaging technologies in an inert environment. This allows wafer-scale and systems-scale fabrication of a wide range of devices including solar cells, batteries and mechanical or thermoelectric energy harvesters.



3D X-Ray CT: for non-destructive *in situ* and 4D studies of composite and buried multilayers, as well as a range of other complex materials systems. It can perform simple analyses such as investigating composition, to more complex experiments such as studying the impacts of temperature, oxidation, wetting, stress, imbibition, drainage and other simulated environmental studies. Specialised loading stages will allow accurate monitoring of 3D deformation processes, such as the swelling of a battery during operation.



Above: CAM-IES launch event at the Maxwell Centre

Centre for Advanced Materials for Integrated Energy Systems (CAM-IES)

The Cambridge Royce has been vital in attracting further funding for energy materials research. In January 2017 the EPSRC awarded £2.1 million networking grant funding to set up the Centre for Advanced Materials for Integrated Energy Systems (CAM-IES), based at the Maxwell Centre and led by Professor Clare Grey.

The Centre is a partnership between four universities: University of Cambridge, Newcastle University, Queen Mary University of London and University College London. The Centre has a strong emphasis on industry engagement and collaborates with many partners including Shell, Tata Steel, Siemens, Sasol, Dyson, and Applied Materials, who engage with the Centre through the funding of collaborative projects. The benefits include direct funding of students, enabling the commercialization of new technologies through giving academic researchers access to specialized equipment and plants for industrial scale-up, and via support of early career researchers through training and expertise in commercialisation of intellectual property.

CAM-IES focuses on the development of advanced materials for energy conversion and energy storage based on:

- solid-state, higher voltage and flow batteries
- solid-oxide fuel cells
- CO_2 gas separation membranes
- hybrid thin film photovoltaics
- large-area thermoelectrics

An overarching goal of CAM-IES is to bring together the UK energy research community via a series of high-visibility networking activities such as road-mapping workshops, pump-priming funding calls, industry engagement events, collaborative short projects, and early career research networking opportunities. Such events allow Winton Scholars and Advanced Research Fellows to develop new collaborations with the UK energy materials community, and to make key links with industrial partners.

For more information about the Cambridge Royce facilities and CAM-IES, please contact Dr Lata Sahonta (sls55@cam.ac.uk)

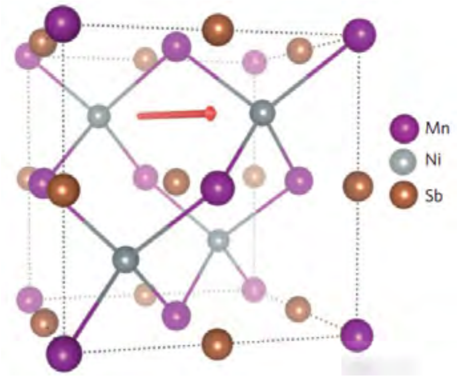
FELLOWSHIPS

Dr Chiara Ciccarelli
Winton Advanced Research Fellow

My research focuses on the question: can we use electricity to write and read the magnetic state of a ferromagnet in an energy efficient and fast way? This is the aim of leading IT companies for the development of the next generation of magnetic random access memories, and it is also a challenge stimulating vibrant research in both experimental and theoretical physics.

In my group we study relativistic effects induced by a special property of the ferromagnet: its unit cell is asymmetric under a space-inversion operations. We demonstrated that these effects allow room temperature control of the magnetic state by an electrical current [Nature Physics **12**, 855-860, 2016]. Vice versa, the same effects allow converting magnetic excitations (magnons) into an easily detectable electrical signal [Nature Nanotechnology **10**, 50-54, 2015].

The question that I will tackle in my recently awarded Royal Society University Research Fellowship is whether these effects can take place on ultra-short timescales, in the order of picoseconds. The timescale is determined by how quickly the magnetic moments can move and in ferromagnets it is pinned to the nanosecond range.



Antiferromagnets offer a way to go beyond this limit since their magnetic dynamics are orders of magnitude faster than in ferromagnets.

Faster timescales also imply that, to study the same relativistic effects, experimental techniques with a sufficient bandwidth must be adopted. Funding from the Winton Programme is giving me the opportunity to build an optical-THz system in the Maxwell Centre in which these studies will be possible. Our laser system recently achieved the emission of 35 femtosecond pulses at the peak power of 1.6 mJ and with a repetition rate of 5 KHz. The set-up will include a 1T electromagnet and a low vibration optical cryostat covering the temperature range 3K-500K.

Two PhD students, Farhan Kholid, who joined the group in October 2016, and

Dominik Hamara, who has just joined us, are currently working on building the set-up, which we aim to have ready in the first quarter of 2018.

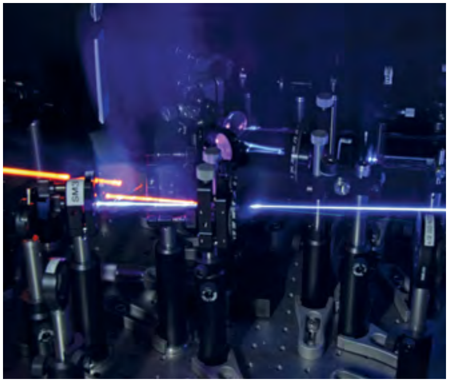
Our collaboration network includes groups expert in ultra-fast spectroscopy such as that of Alexey Kimel and Theo Rasing in Nijmegen, with which we shared a Leverhulme International Network grant in 2015 and with which we have an open European COST and a European FET applications, but also theory groups such as the group of Tomas Jungwirth in Prague. The antiferromagnetic materials that we will measure come from several groups: the group of Claudia Felser in Dresden, the group of Brian Gallagher in Nottingham and, in Cambridge, the groups of Russell Cowburn and Jason Robinson, with whom I am also co-supervising a Winton Scholar and NanoDTC student Lauren McKenzie-Sell.

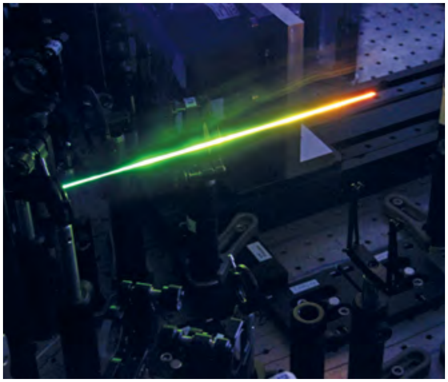
Dr Felix Deschler
Winton Advanced Research Fellow

The discovery of semiconducting materials with high luminescence yields is key for the development of efficient optoelectronic and photonic applications, yet there is no general understanding of the underlying design rules. My research investigates how the structure of semiconductor materials controls the properties and dynamics of excited states, with the goal of translating these principles into novel, sustainable optoelectronic applications.

We are currently exploring the connection between excited state dynamics and local structural properties, with the aim of understanding the recombination dynamics of highly-luminescent materials. For this, we use advanced ultrafast spectroscopy and diffraction experiments in our research labs and at national facilities. Previous studies typically reported spatially-averaged information on the excited state recombination of a material, which cannot give a full picture of the dynamics. In our new approach, we now aim to look at the photon emission process at a much more local level by developing a spectroscopic setup that will push the limits in time and spatial resolution by an order of magnitude.

Our results will generate design rules to discover novel efficient materials for light-emitting diodes and solar cells.





During my first months as a Winton Fellow I have recruited four PhD students, Haralds Abolins (Winton Scholar), Sean Bourelle (Graphene CDT), Sascha Feldmann (DFG Studienstiftung) and Tim van de Goor (nanoDTC). In addition, two post-doctoral researchers, Dr. Haizhou Lu (Fudan University) and Dr. Ravichandran Shivanna (Royal Society Newton Fellow), currently work in the group.

Through existing collaborations at the Politecnico di Milano (Prof. Giulio Cerullo) I have recently explored the speed limits of carrier-carrier interactions in hybrid perovskites [Richter, Nat Comms, 8, 15976, 2017]. I have further established new collaborations with groups at Stanford University (Prof. Aaron Lindenberg), and also within Cambridge University (Prof. Oren Scherman, Dept. of Chemistry).

Figures, left to right:

Inversion asymmetric unit cell of ferromagnet NiMnSb, which we have used in our studies on electrically induced magnetic torques.

Work in progress in the Maxwell Centre laboratories. We are building an optical-THz setup to study spintronics effects at the picosecond timescale.

Image of the advanced spectroscopy facilities used for ultrafast probing of photoexcited states dynamics in novel semiconductor materials.

FELLOWSHIPS

Alpha Lee
Winton Advanced Research Fellow

My group focuses on using machine learning to discover functional soft materials such as organic electrolytes and bioactive molecules. Recent technological advances have made high-throughput simulations and experiments of soft matter within reach. Our vision is to integrate the underlying physics into machine learning of large datasets.

Ionic liquids – room temperature molten salts – are used in the industry as electrolytes for supercapacitors and batteries. Despite their ubiquity, designing ionic liquids to maximize the capacitance and power of supercapacitors remains a key challenge. Using systematic experimental and theoretical studies of the correlation length in concentrated electrolytes, we derived a scaling picture for the structure of the bulk liquid [1]. We have also contributed mechanistic insights into charge storage in supercapacitors [2] and ions under nanoconfinement [3]. The next step for our group is to connect the molecular chemistry of organic electrolytes to condensed phase properties to enable *in silico* rational design, addressing problems such as finding the optimal ion-solvent-electrode combination for supercapacitors. The challenge of devising informative representations of organic molecules is similarly salient in the design of small molecule drugs. We have made some recent progress in this area, applying techniques from random matrix theory to distill important chemical features that contribute to the potency of a molecule [4]. Going forward, we aim tackle challenges such as predicting hydration free energy, protein-ligand binding free energy, and synthetic accessibility of organic molecules, ultimately arriving at an automated workflow for preclinical drug discovery.

Above: Squeezing in ion and solvent molecules inside a nanoslit, a simplified model for charge storage in nanoporous supercapacitors, is analogous to trying to pack smaller apples and larger oranges in a fruit box. The characteristic size of an ion-pair is larger than typical organic solvent molecules, and this geometric mismatch induces non-trivial physics. We showed that structure of the underlying packing changes abruptly as the electrolyte composition is varied [3].

The methodology that we are advancing is a three-pronged workflow, combining model selection, model design and experiment design. We aim to develop scalable Bayesian models that can also predict their own uncertainty. This will enable us to go beyond heuristics and develop a statistically optimal strategy to select between different modeling strategies, balancing between model uncertainty and computational effort. In terms of model design, we aim to design machine-learning models that incorporate physics as inductive bias. Finally, we aim to use machine-learning models to design high-throughput experiments to optimally infer model parameters. We have recently published a model showing how to combine easy-to-acquire qualitative data with much fewer expensive quantitative data to arrive at an accurate quantitative model [5].

Since arriving in Cambridge in September 2017, I was joined by four MPhil and MSci students working on projects pertaining to machine learning and soft materials. I am also co-supervising Bill Stockham (PhD student from NanoDTC) on designing enzyme-inspired DNA origami catalysts. We collaborate with the experimental groups of Dr Erika Eiser in Optoelectronics, Profs Clare Grey and Matthew Gaunt in Chemistry, and Professor Susan Perkin in the Department of Chemistry, University of Oxford.

[1] A. A. Lee et al., Physical Review Letters, 119, 26002 (2017)
[2] A. A. Lee et al., Physical Review X, 6, 21034 (2016)
[3] A. M. Smith, A. A. Lee and S. Perkin, Physical Review Letters, 118, 096002 (2017)
[4] A. A. Lee et al., Proceedings of the National Academy of Sciences, 111, 13564 (2016)
[5] A. A. Lee et al., Physical Review Letters, accepted (2017) [arXiv:1702.06001]

AFFILIATED LECTURER

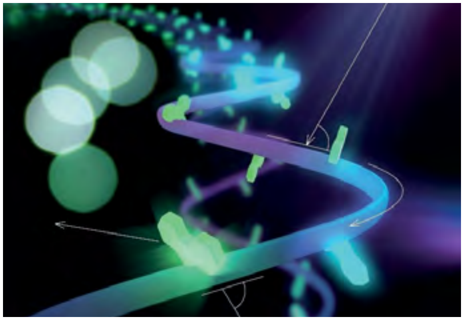
Dr Hugo Bronstein
Winton Affiliated Lecturer

Research in my group involves the synthesis of novel conjugated materials for use in organic optoelectronic devices such as solar cells, light emitting diodes and transistors. We are particularly interested in synthesizing materials that help understand and utilise triplet excited states, for example singlet fission, upconversion, reverse intersystem crossing, due to their unique and fascinating properties.

Our aim is to begin the research process from the "bottom up". By developing a true understanding of the fundamental properties of conjugated materials, simultaneous advances will be made across all areas of conjugated polymer research and its relevant applications.

There are a few key properties of conjugated polymers which are important across ALL applications which, if they could be controlled, would offer rapid advances across all fields of research. For instance, it can be argued that in applications where there is interaction between light and matter, the three most important of these properties are: excited state energy, lifetime and diffusion length.

Conjugated polymers have two types of excited states: singlets and triplets. Singlet excited states are generated by quantum mechanically allowed transitions responsible for light absorption and emission and typically have very short lifetimes. On the other hand, absorption and emission to and from triplet excited states are quantum mechanically forbidden and so they have much longer lifetimes. It has been speculated that the longer lifetime of the triplet excited state could be used to enhance the performance of organic solar cells by allowing more time to harness the power of this exciton. However, due to the difficulty in generating and measuring the properties of the triplet excited state, not much is known about their fundamental properties.



We have recently synthesized a series of conjugated polymers which allowed the measurement of the singlet-triplet energy gap and its diffusion length. Both of these parameters have long been discussed in the literature but rarely measured in the laboratory. By judicious incorporation of a small amount of a heavy-metal containing complex into the conjugated polymer backbone we have been able to generate exclusively triplet excited states along the polymer backbone. [1]

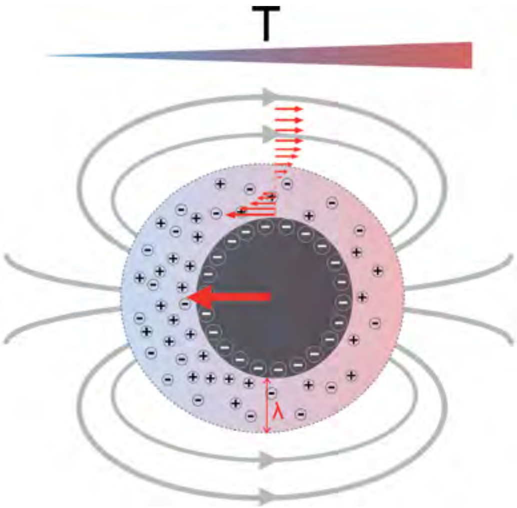
Going further we then synthesized an entirely new class of conjugated polymer where we reduced the energy gap between the singlet and triplet excited states. This was done by introducing orthogonal electron accepting groups onto the polymer backbone, thus reducing the overlap between ground and excited states. The outcome was a new class of material which would rapidly generate triplet states, which were then able to be thermally populated back into the singlet state for light emission. This new class of materials is anticipated to have application in solar cells with drastically reduced loss mechanisms and organic photocatalysis. [2]

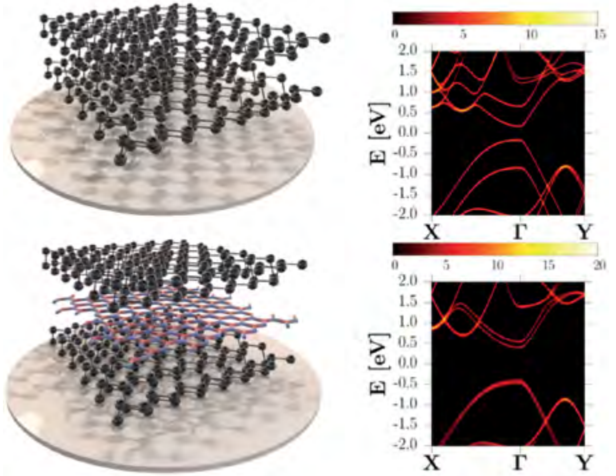
In order to develop these and other novel conjugated materials from proof-of-principle into actual applications they must firstly be understood at a fundamental level, and then they must be incorporated into actual devices. For this the Winton Programme and the Maxwell Centre are the ideal place where synthetic chemists, spectroscopists, device physicists and theorists can all interact to develop a new generation of optoelectronic device.

[1] Synthesis and Exciton Dynamics of Triplet Sensitized Conjugated Polymers. R. Andernach, H. Utzat, S. D. Dimitrov, I. McCulloch, M. Heeney, J. R. Durrant, H. Bronstein
J. Am. Chem. Soc. 2015, 137, 10383-10390,
[2] Synthesis and Exciton Dynamics of Donor-Orthogonal Acceptor Conjugated Polymers: Reducing the Singlet-Triplet Energy Gap. D. M. E. Freeman, A. J. Musse , J. M. Frost, H. L. Stern, A. K. Forster, K. J. Fallon, A. G. Rapidis, F. Cacialli, I. McCulloch, T. M. Clarke, R. H. Friend, H. Bronstein
J. Am. Chem. Soc., 2017, 139, 11073–11080

Above: Donor-orthogonal acceptor conjugated polymer capable of emitting light through thermally activated delayed fluorescence

SCHOLARSHIPS
Cohort starting 2014/15





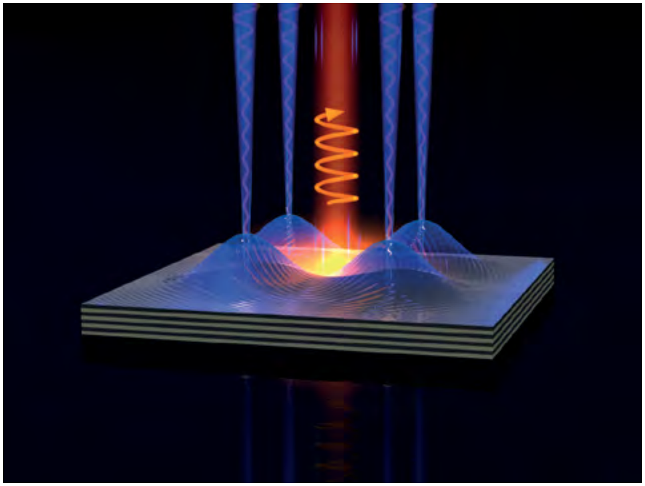
Jerome Burelbach's research is on thermophoresis, the motion of colloids or biomolecules in a temperature gradient. Thermophoresis has uncovered a large number of applications, ranging from thermal separation techniques and biophysical analysis to the study of conditions that facilitated the formation of life. Having developed an experimental technique for bias-free measurements of colloidal thermophoresis, he focussed on the theoretical description of the effect, a topic of intense research that has been heavily debated in recent literature. Jerome has been particularly interested in developing a consistent theoretical model based on Onsager's theory of Non-Equilibrium Thermodynamics (NET) and its validation by means of computer simulations. For this purpose, he implemented a mesoscale-molecular dynamics scheme known as Multi-Particle Collision Dynamics, which has allowed him to test the range of validity of his theoretical model and to quantify the deviations from NET resulting from fluid advection at the colloidal interface.

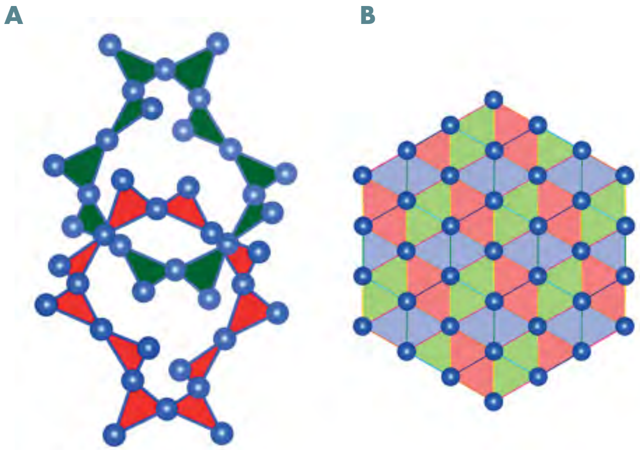
Above: Schematic depiction of hydrodynamic stresses caused by a temperature gradient inside the electric double layer of a charged colloid.

Gabriel Constantinescu's research is aimed at two-dimensional heterostructures, which are stacks of layered materials only a few nanometers thick. With such a vast number of possibilities, the most practical option is to study them computationally. Gabriel develops and uses linear-scaling software that can describe these large nanostructures, and has already successfully simulated their spectroscopic and quantum transport properties (Nano Letters **16,** 2586, 2016).

Moreover, he is developing a new formalism for calculating vibrational properties in large systems, which can further contribute to understanding these heterostructures. The goal is to understand which combination of layered materials ensures the desired properties of future nanoelectronic devices.

Above: Bandstructures of black-phosphorus layered interfaces, with applications in optoelectronics.





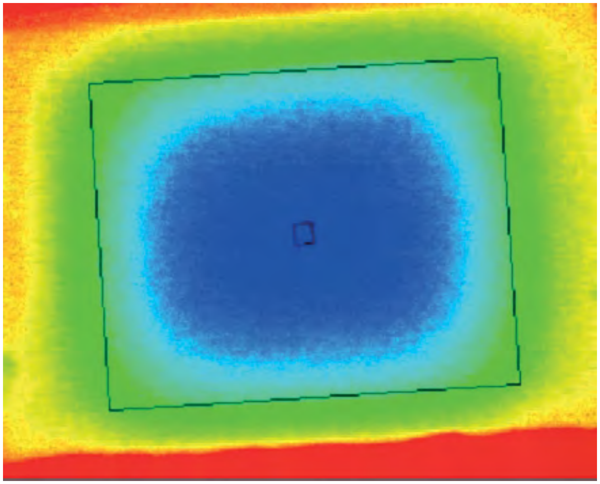
Yago del Valle-Inclan Redondo works on optical control in high-quality GaAs microcavities, where the fundamental excitations of the system are mixed light-matter particles called exciton polaritons. Under non-resonant excitations, polaritons thermalise into macroscopically occupied quantum states - polariton condensates.

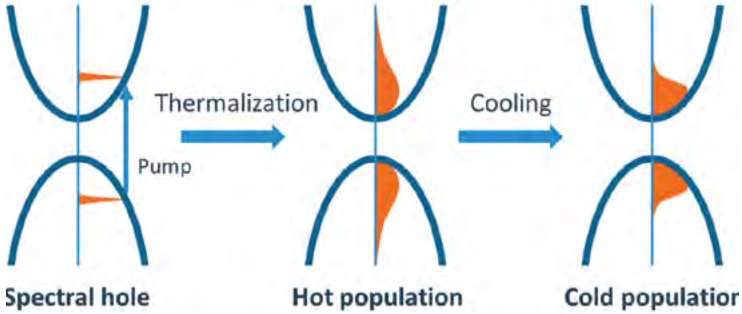
Yago's research focuses on using spatially patterned non-resonant laser fields to control polariton condensates. It has been demonstrated that it is possible to create trapped condensates with unexpected spin properties, allowing them to create a sub-fJ electrical spin switch and shedding new light into the spin relaxation mechanisms of polaritons. Building on this work, the possibility has been demonstrated of creating and controlling the coupling between many trapped polariton condensates, paving the way to using polariton lattices for quantum simulation.

Above: Four non-resonant, linearly polarised laser beams (blue) create a trapped condensate emitting circularly polarised light (orange).

Paromita Mukherjee's research focuses on investigating new magnetic refrigerants for cooling to temperatures near absolute zero. Many areas of fundamental and applied scientific research and devices such as magnetic resonance imaging scanners and cryogenic sensors require cooling to such low temperatures. Traditionally this has been achieved using non-renewable liquid helium which is becoming increasingly scarce and expensive. A sustainable alternative is magnetic refrigeration using geometrically frustrated magnetic materials, where the structural geometry prevents the pairwise magnetic interactions from being satisfied simultaneously. She is studying the fundamental magnetic properties and magnetic refrigeration efficiency of different families of frustrated lanthanide oxides and has found promising candidates for low temperature magnetic cooling in the lanthanide garnets and lanthanide borates.

Above: Geometrically frustrated magnetic lattices: a) Lanthanide garnets; b) Lanthanide borates.





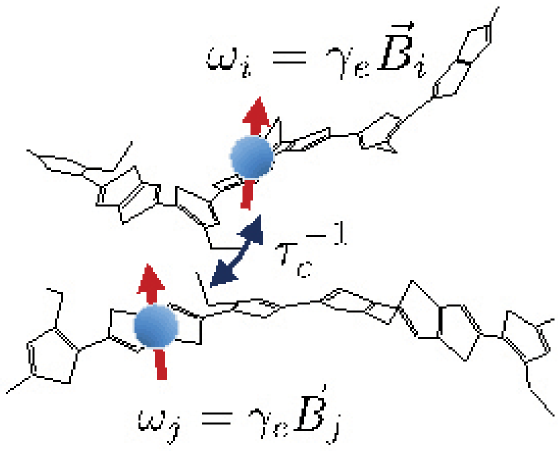
Bhaskaran Nair is interested in the development of novel electrocaloric materials that can be exploited in prototype refrigerators. Electrocaloric effects are generally found near phase transitions that couple to electric fields and are therefore most often found in ferroelectrics. However, electrocaloric effects in ferroelectrics are generally limited by a tradeoff between size and breakdown field strength that poses a challenge for developing electrocaloric refrigeration. Bhaskaran's work also explores the extension of electrocaloric effects to new materials systems exhibiting phase transitions that couple to the electric field by a change in charge transport behavior. Such effects would take the system far away from equilibrium, going beyond the purview of (near) equilibrium thermodynamics used to describe electrocaloric effects and thermoelectric effects.

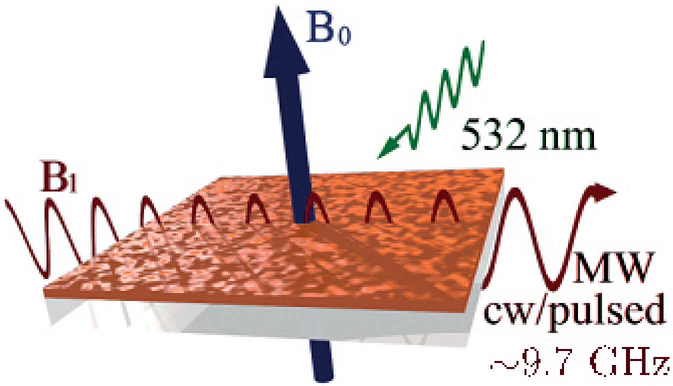
Above: Thermal imaging of electrocaloric effects

Johannes Richter is investigating halide perovskite solar cells, which have shown efficiencies close to those of silicon solar cells after only 5 years of research. At the same time, solution processing allows low-cost manufacturing of perovskite-based solar cells and LEDs.

Johannes is studying the early-time carrier relaxation in perovskites after sunlight absorption using ultrafast spectroscopy. He recently measured for the first time the ultrafast timescales on which electrons in perovskites scatter and exchange energy - 10 quadrillionths of a second. This process is ultimately limiting the time for extraction in hot carrier solar cells. Furthermore, his research has shown how light out-coupling problems limit solar cell and LED efficiency and he demonstrated how surface roughness can help to overcome these limitations.

Above: Charge carrier relaxation after light absorption in perovskite semiconductors





Sam Schott's research focuses on using organic semiconductors as materials systems for spin electronics (spintronics). These carbon-based materials provide a rich variability of structures and show exceptionally long spin life-times but little is known about their spin physics.

To this end, Sam has investigated the coupling of a charge's orbital motion to its spin in a range of isolated, doped molecules and has shown that this spin orbit coupling can be tuned over orders of magnitude through changes in the molecular geometry and resulting shifts of the spin density distribution (Nat. Comm. 8, 15200, (2017)).

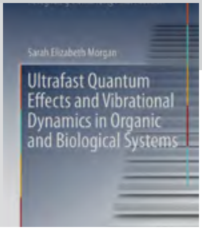
Currently, Sam is exploring the effect of charge motion on spin dephasing in a series of high mobility polymers relevant for device applications.

Above: Illustration of spin hopping between polymer chains and sampling different local magnetic environments.

Leah Weiss has used spin to probe the dynamics of singlet fission, a process with the potential to boost the efficiency of solar energy generation. This process allows a light-induced spin-0 excitation in one molecule to split, forming a pair of lower energy spin-1, triplet, excitations over two molecules. This multiplication process could be integrated with silicon technologies to enable more efficient use of the solar spectrum. Spin plays a key role in the kinetics of these pair states. Using microwave manipulation and optical luminescence in external magnetic fields, Leah's work has demonstrated that triplets can form strongly interacting pairs, which evolve to form stable, high-spin quintet states, remaining bound over long timescales. These results have highlighted the importance of intermolecular structure and interactions in the dynamics of singlet fission.

Above: Schematic of electron spin resonance experiments on films of organic semiconductors using microwave and optical photons in an external magnetic field.

PROGRAMME HIGHLIGHTS

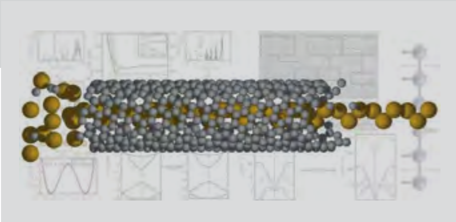


Quantum Biology and ultrafast quantum dynamics in organic molecules research wins Springer Thesis Prize

Winton Scholar Dr Sarah Morgan won this year's prestigious Springer Thesis Prizes for doctoral research. The award, which led to the publication of Sarah's PhD thesis, was made in recognition of her work on the nascent field of quantum effects in biological systems and how these might be harnessed in future light-harvesting technologies based on organic materials.

The work, supervised by Winton Advanced Research Fellow Dr Alex Chin, contains some of the first theoretical studies of how the quantum mechanics of molecular vibrations can impact the efficiency of light-capturing optoelectronic processes, and also how the structural coordination of folded protein networks enable vibrational disturbances to be communicated between functional sites.

Sarah's thesis is now available as an E-book, here: https://link.springer.com/book/10.1007/978-3-319-63399-2.

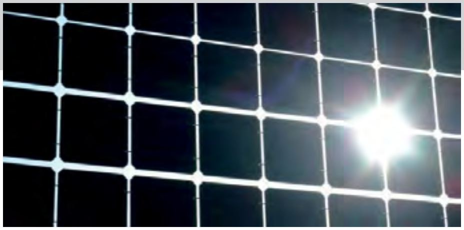


Scientists construct a stable one-dimensional metallic material

A research team led by Winton Advanced Research Fellow, Dr Andrew Morris has developed the world's thinnest metallic nanowire, which could be used to miniaturise many of the electronic components we use every day. With collaborators Dr Jeremy Sloan and Dr David Quigley at University of Warwick, they have developed a wire made from a single string of tellurium atoms, making it a true one-dimensional material. These one-dimensional wires are produced inside extremely thin carbon nanotubes (CNTs) – hollow cylinders made of carbon atoms that are nm in diameter.

Results reported this year [ACS Nano, **11**, 6, p6178, 2017] have also shown that it is possible to alter the shape and electronic behaviour of the nanowires by varying the diameters of the tubes which encapsulate them.

www.cam.ac.uk/research/news/scientists-construct-a-stable-one-dimensional-metallic-material



10 quadrillionths of a second time limit for ultrafast perovskite solar cells

Researchers in the Optoelectronics group at the Cavendish and at the Politecnico di Milano in Italy have quantified the astonishingly high speeds at which future solar cells would have to operate in order to stretch what are presently seen as natural limits to their energy conversion efficiency.

The study investigated photovoltaic devices based on perovskite materials, the results being published in Nature Communications [8, 376, 2017] with Winton Scholar, Johannes Richter as lead author.

Moving electrons at this ultrafast rate would enable the creation of "hot carrier" cells. These are solar cells which can generate electricity more efficiently by making use of the added kinetic energy that electrons have for a brief moment just after they are created, while they are moving at high speed.

www.cam.ac.uk/research/news/10-quadrillionths-of-a-second-to-extraction-researchers-set-time-limit-for-ultrafast-perovskite

Image above © James Cridland, via Flickr

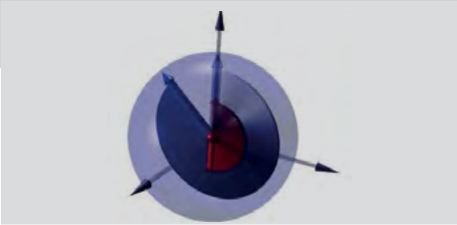
World's smallest magnifying glass

Using gold nanoparticles, researchers have concentrated light down to dimensions smaller than a single atom, enabling them to study individual chemical bonds inside molecules, and opening up new ways to study light and matter.

Research in the Nanophotonics Group at the Cavendish Laboratory led by Professor Jeremy Baumberg in collaboration with colleagues from Spain have created the world's smallest magnifying glass which focuses light a billion times more tightly, down to the scale of single atoms.

The results, reported in the journal Science [354, 6313, 2016], with lead author Winton Scholar, Felix Benz, open up new ways of studying the interaction of light and matter, including the possibility of making the molecules in the cavity undergo new types of chemical reactions, which could enable the development of entirely new types of sensors.

www.cam.ac.uk/research/news/worlds-smallest-magnifying-glass-makes-it-possible-to-see-individual-chemical-bonds-between-atoms



Researchers road-test powerful method for studying singlet fission

The singlet fission process creates two excitons from a single photon, doubling the number of charges that can be generated. This can produce solar cells that will be much more energy efficient, but the process needs to be fully understood in order to optimize the performance.

Winton Scholar, Leah Weiss, is lead author on a Nature Physics paper [**13**, 171-181, 2017] that describes a powerful technique for studying electrons generated through singlet fission. Their approach employed lasers, microwave radiation and magnetic fields to analyse the spins of excitons, which are energetically excited particles formed in molecular systems.

Beyond trying to improve photovoltaic technologies, the research also has implications for wider efforts to create fast and efficient electronics using spin, so-called "spintronic" devices, which rely on being able to measure and control the spin properties of electrons.

www.cam.ac.uk/research/news/researchers-road-test-powerful-method-for-studying-singlet-fission

Akshay Rao wins 2017 IOP Henry Moseley Award and Prize

Winton Advanced Research Fellow, Dr Akshay Rao was awarded by the Institute of Physics the Henry Moseley Award and Prize for his pivotal research in the field of organic semiconductors and the role of spin in the operation of solar cells.

Akshay's principal concern has been the fission of a spin-singlet photoexcitation in an organic semiconductor into a pair of spin-triplet excitons. This process is spin-allowed and energetically allowed when the exchange matches half of the singlet energy, as found in materials including pentacene.

Akshay showed that the triplet exciton can be ionised to an electron–hole pair at a suitable heterojunction, and that the triplet exciton can be rapidly tunnelled into an inorganic semiconductor. This has established the scope to use this process of exciton doubling to couple to practical solar cells, and may be able to deliver tandem-cell performance in a cheap single-junction cell.

PUMP PRIME

Funding of up to £50k is available to seed new research projects within Physics as well as in partnership with other departments. These projects have enabled a number of new collaborations to be set up, often leading to longer term activities and follow on funding from other sources. Some examples are provided here of pump prime projects. Further information and application details can be found at www.winton.phy.cam.ac.uk/pumpprime

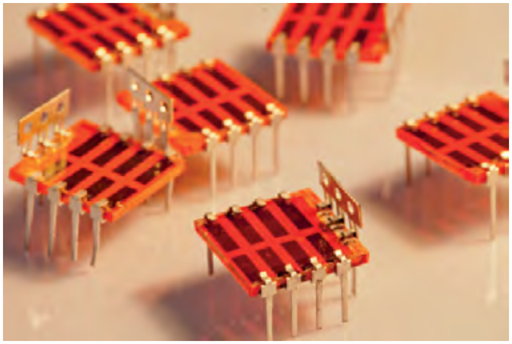
Exploring new, all-inorganic BiO-based compounds for planar heterojunction (PHJ) solar cells

Professor Judith Driscoll, Department of Materials Science and Metallurgy and Dr Robert Hoye, Optoelectronics Group

The thin-film photovoltaics field has recently been revolutionised by the advent of hybrid lead-halide perovskites, which have achieved unprecedented rises in efficiency to 22.1% after only five years of research. The lead content however remains a concern for wide-scale deployment, and non-toxic alternatives urgently need to be identified and developed. Non-toxic bismuth-based compounds are potential replacements.

Our project has explored bismuth oxyhalide (BiOI) materials. Halides have relatively low melting points enabling easy processability, and oxyhalides are better than pure halides since they are more stable in air. Also, bismuth-based materials may replicate the tolerance of lead-halide perovskites to defects. Indeed, using theory we found bismuth oxyiodide to be tolerant towards a range of defects. From a physical point of view, BiOI has a suitable bandgap to work in tandem with silicon.

We grew dense thin films using a vapour deposition method and found them to be stable in air for at least 197 days. We developed thin film solar cells by sandwiching bismuth oxyiodide between two stable oxide layers to

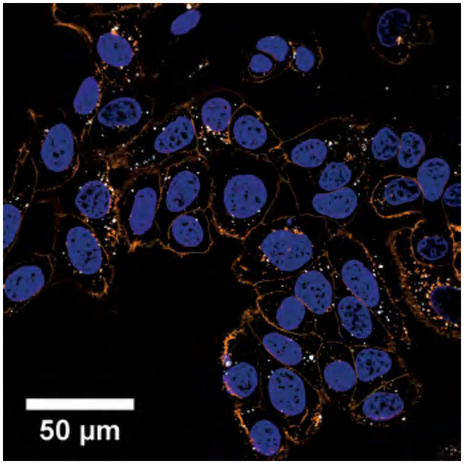


selectively extract photogenerated charge. The efficiencies exceeded not only previous reports of solar cells based on this material, but also other recently-explored bismuth halides and chalcohalides.

Open questions in oxidative stress biology

Dr Sarah Bohndiek (Biological and Soft Systems Group) and Professor Mete Atatüre and Dr Helena Knowles (Atomic, Mesoscopic and Optical Physics Group)

This project combines sensing of the intracellular environment (based on diamond spins) with sensing of the cellular biochemistry (based on Raman spectroscopy) to evaluate oxidative stress conditions in cancer cells. Oxidative stress, referring to an imbalance of damaging reactive oxygen species (ROS) and compensating antioxidants in cells, is a key marker in the incidence and progression of several diseases, including cancer. Current methods for the evaluation of oxidative stress take bulk

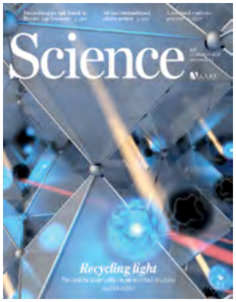


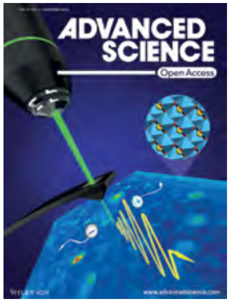
measurements of millions of cells and so have limited sensitivity to the heterogeneity of cellular responses. Through the course of this project, we created a unique microscope that enables for the first time non-toxic, real-time measurements of the chemical and environmental response to oxidative stress at the single cell level. We have thoroughly characterised the technical performance of this microscope, and applied it to evaluate the impact of different fluid environments on the fluorescence response of nanodiamonds. We have also quantitatively determined the biological impact of nanodiamonds in cultured cancer cells (see Figure). We are currently progressing towards measurement of oxidative stress in live cells, targeting cancer cells with different chemotherapy drugs. Ultimately, making such measurements could open opportunities for early identification of drug response and resistance, optimising treatment for cancer patients.

Excited state diffusion in hybrid nano-structures

Dr Felix Deschler (Optoelectronics Group) and Dr Hannah Joyce (Department of Electrical Engineering)

This grant provided funding for experimental facilities to study spatial excitation dynamics in hybrid perovskite materials. The unique insights from our experiments allowed us to make key advances in the understanding of excited state recombination in this disruptive material class for optoelectronics. We discovered that absorbed photons can be 'recycled', which puts the potential of hybrid perovskites on par with the highest performing semiconductor materials to date [Pazos-Outón et al, Science, **325**, 6280, p1430, 2016 and Vrucinic et al, Advanced Science, **2**, 1500136, 2015]. The funds further initiated investigations of single-crystalline perovskite nanostructures, for which we initially developed nanowires with high purity and controlled properties. Our first results on the excited states dynamics in these systems suggest that confinement effects have a surprisingly small impact on carrier lifetimes, and that





large gains in recombination efficiencies are likely in lasing and LED structures. In a next step, we will implement these structures in electrically driven prototype devices.

Images, left to right:

Researchers have made a leap-forward in the exploration of bismuth-based solar cells, identifying bismuth oxyiodide to be air-stable and tolerant towards defects. (Image credit: Steve Penney).

Nanodiamonds are endocytozed into breast cancer cells. Blue is NucBlue nuclear stain, orange is WGA-AF488 cell membrane cell, white shows the nanodiamonds (both individual and as aggregates) inside MDA-MB-231 breast cancer cells in vitro. This image is taken after 48 hours under a diamond exposure of 1µg/ml.

WINTON EVENTS

Winton Symposium on Solar Energies

The fifth Winton Symposium was held last year on the topic of 'Solar Energies' with the aim of exploring the underlying science of light harvesting and how this may lead to further advances in performance. Successful deployment at the global scale requires engagement with the commercial world, a theme that was also touched upon by the speakers.

Professor Sir David King, the UK's Foreign Secretary's Special Representative for Climate Change provided an overview of the Paris agreement that has committed to limiting average global temperature rise to below 2 degrees, preferably less than 1.5 degrees. Even if these targets are met there are considerable risks of significant impact from rising sea levels and crop failures. Meeting this target requires rapid growth of clean energy on a global scale for which he has helped establish the Mission Innovate Programme, with twenty-two major governments committed to doubling their governmental clean energy RD&D over the next five years. This provides a great opportunity for scientists to come together to find solutions to our pressing needs.

Professor Greg Engel from the University of Chicago explored what we can learn from biology where photosynthesis has evolved over billions of years to produce a highly effective method of harvesting light. His group uses ultrafast spectroscopy to study the dynamics of protein complexes that have precisely placed chromophores to produce highly efficient light harvesting antenna that coherently couple to reaction centres. His work aims to understand the design principles that influence the coherence and thereby develop strategies for making more efficient devices.

Professor Albert Polman from the FOM Institute AMOLF in Amsterdam explained the Schockley-Queisser limit that defines the theoretical limit for the efficiency of single junction solar cells. In practice cells are not able to reach this limit due to losses that can be described in terms of carrier management, which is mainly a material science problem, and light management which is failing to collect and capture incident light. He described a number of examples of how nano-structuring can re-direct light to improve the amount of captured light and thereby efficiency in a cost effective manner.

Professor Tonio Buonassisi from MIT calculated that we need 4-5 TW of new installed solar energy by 2030 to meet the Intergovernmental Panel on Climate Change (IPCC) targets, whilst existing capacity can only produce 1 TW. To manage this shortfall 22% annual growth will be needed in manufacturing capacity. To meet these challenging targets, he advocated that innovation is needed to drive costs further down by reducing the capital expense of the manufacturing plants and increasing the efficiency of solar cells. His group is working on the latter through developing lower defect materials and optimising tandem cells.

Dr Frank Dimroth from the Fraunhofer Institute for Solar Energy Systems in Freiburg has led research that has produced multi-junction III/V solar cells that reached 46.1% efficiency. These III/V materials are more expenses per unit area than Si, but with solar concentrators these systems can become more cost effective and have been successfully deployed in South Africa where a 44MW system is operating. One of the challenges for these cells is building multi-junctions for which his group have developed wafer scale bonding techniques.

Professor Henry Snaith, Department of Physics, Oxford University provided an overview of solar cells made with organometallic lead halide perovskite semiconductors. Work of his group has taken these to efficiency levels up to 22% approaching those of silicon, in the space of 5 years. The big surprise is that these materials can operate in solar cells with much higher levels of impurities than can be tolerated in silicon, and this makes it possible to process the materials very cheaply. There are barriers yet to be overcome in regard to stability of the materials but these are very promising candidates for combining with Si to make efficient tandem cells, which is being commercialised by their spinout company Oxford PV.

Professor Jenny Nelson, Professor of Physics at Imperial College, talked about solar cells made with organic molecular semiconductors. The organic materials can be processed from solution, such as by direct printing, and so offer the opportunity to move to low cost and low energy production. There has been considerable progress in optimising these materials for solar harvesting, both through manipulating the electronic properties of these molecules through their chemistry, and through creating different microstructures in polymer blend films. Efficiencies have now reached 11.5%, with research on-going to understand the sources of energy losses in order to push efficiencies to the levels needed to be competitive with other technologies.

See also article by Professor Richard Jones - "Optimism - and realism - about solar energy" www.softmachines.org/wordpress/?p=1940

Above, left to right:

Professor Sir David King addresses the audience at the Winton Symposium at the Cavendish Laboratory; Professor Henry Snaith; Professor Jenny Nelson.

PEOPLE

Alessio Caciagli, Alex Welbourne, Antonis Alvertis, Bhaskaran Nair, Dédalo Sanz-Hernández, Di Jin, Dr Akshay Rao, Dr Alessandro Rossi, Dr Alex Chin, Dr Alpha Lee, Dr Amalio Fernández-Pacheco, Dr Andreas Nunnenkamp

Dr Andrew Morris, Dr Chiara Ciccarelli, Dr Erika Eiser, Dr Felix Deschler, Dr Hannah Joyce, Dr Hugo Bronstein, Dr Nalin Patel, Dr Ottavio Croze, Dr Robert Hoye, Dr Rosana Collepardo, Dr Sam Stranks, Dr Sarah Bohndiek

Dr Siân Dutton, Dr Silvia Vignolini, Dr Suchitra Sebastian, Dr Tijmen Euser, Evelyn Hamilton, Ezequiel Rodriguez Chiacchio, Florian Schroeder, Gabriel Constantinescu, Hajime Shirohara, Hannah Laeverenz Schlogelhofer, Hope Bretscher, Jan Beitner.

Jannes Gladrow, Jerome Burelbach, Jesse Allardice, Johannes Richter, Lauren McKenzie-Sell, Leah Weiss, Martin Mayo, Paromita Mukherjee, Prof Alison Smith, Prof Clare Grey, Prof Erwin Reisner, Prof Henning Sirringhaus

Prof Jason Robinson, Prof Jeremy Baumberg, Prof Judith Driscoll, Prof Mete Atatüre, Prof Neil Mathur, Prof Pietro Cicuta, Prof Richard Friend, Prof Stafford Withington, Prof Tuomas Knowles, Prof Ulrich Keyser, Raj Pandya, Sam Schott

Sean Cormier, Sivapalan Chelvaniththilan, Sofia Taylor, Theresa Jakuszeit, Tianheng Zhao, Tobias Wenzel, Ture Hinrichsen, Virgil Andrei, Wenting Wang, Yago del Valle-Inclan Redondo, Zachary Ruff, Zahra Andaji-Garmaroudi

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Professor Andy Parker
Head, Department of Physics,
University of Cambridge

In attendance:
Professor Lindsay Greer
Head, School of the Physical Sciences,
University of Cambridge

THE WINTON PROGRAMME FOR THE

Physics of Sustainability

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