UNIVERSITY OF CAMBRIDGE

THE WINTON PROGRAMME FOR THE

Physics of Sustainability

ANNUAL REPORT

2016

The Winton Programme for the Physics of Sustainability began with a £20 million donation by David Harding and has now been operating for five years, during which the Programme has invested in numerous research topics related to sustainability.

The funds continue to support and attract bright researchers from across the globe, with the Maxell Centre providing a base for the Winton community and space for new state-of-the-art research facilities to assist their research. This report provides an overview of the activities of the Programme and some of the highlights of the year.

REVIEW

Richard Friend,
Cavendish Professor of Physics

The Winton research community is now brought together in the Maxwell Centre, where we have a range of state-of-the-art research laboratories, and attractive office/social space designed to bring everyone in the building together. This moves us to a new phase. The Winton research community is diverse and it will be exciting to see when chance conversations across non-intersecting research areas spark new ideas and identify new possibilities. The Maxwell Centre was designed to be a hub for research across the whole of West Cambridge and we are really pleased to see that it is already drawing researchers in from across the whole site, not just for the excellent coffee, but also to meet and to discuss science.

We had always intended that the Winton Programme would allow us to explore new ways to support research. So, the laboratory space in the Maxwell Centre is being set up to operate as a set of user facilities that support both expert users and also those who want to try out techniques new to them. Support from the Winton Programme has underpinned much of what we have been able to set in place, and we have also brought in support from the Engineering and Physical Sciences Research Council, and from the European Research Council. The 'Materials Characterisation' suite is now fully functional and provides vastly improved facilities for measurements of structure and of electrical and magnetic properties, down to very low temperature and up to very high magnetic fields. New laboratories for optical spectroscopy with time resolutions down towards 10 fsecs, and for opto-fluidics are now fully functional and support a large user base. During 2017 research facilities provided for the Sir Henry Royce Institute for Advanced Materials, for growth and characterisation of materials and devices, will bring the Maxwell Centre to full capacity.

This year's Symposium focusses on the science that underpins future prospects for solar cells. Silicon-based photovoltaic technology has dropped in price much faster than expected, by a factor of ten within not much more than a decade, and in the right parts of the world, feeds electricity into the grid at costs lower even than from 'fracked gas' generation. However, there are real prospects to raise the efficiency and lower the cost of large-scale solar cells way beyond current technology, as the Symposium will explore.

PROGRAMME UPDATE

Nalin Patel, Programme Manager

Overview

The Winton Programme for the Physics of Sustainability is now in its fifth year of operation. The Programme continues to support a 'bottom-up' approach to exploring new areas of science through appointments of Scholars and Fellows and seed funding new ideas through pump-priming grants. This year, with the launch of the Maxwell Centre there have been opportunities to support more 'top-down' activities through increased investment in infrastructure and Departmental Lecturers. The combination of people and infrastructure investment will make the Winton Programme well placed to tackle the basic science that has the potential to lead to the breakthroughs necessary to meet the growing demands for natural resources.

Programme Activities

The Programme continues to attract and support bright students and researchers through the annual Winton Scholarship and Winton Advanced Research Fellowship schemes. This year eight Scholars were appointed, bringing the total to date of thirty-seven - details of this fifth cohort of PhD students is provided on the opposite page. The Scholarship scheme is open to applicants from around the world, and within the latest cohort we have students from Australia, Canada and Venezuela.

The latest Winton Fellowship was awarded to Rosana Collepardo-Guevara; a description of her research being provided later in the report. Her appointment brings the total number of Winton Fellows to eight – their research covers topics ranging from battery materials, quantum biology, materials computation, algal biofuels, magnetic microstructures and photovoltaics.

The Programme has awarded a further three Winton Pump Prime grants this year, bringing the total to eighteen. Many of the projects have fostered collaborations between the Cavendish Laboratory and other departments across the University and have led to more substantial follow-on funding.

Maxwell Centre

Much of the activity of the Winton Programme has transferred to the Maxwell Centre, which is housed in the new building on the West Cambridge site next to the Cavendish. The majority of the Fellows now have their offices and laboratory space within the Centre, offering increased opportunities for interactions within the Winton community as well as with the other occupants from a range of disciplines. Further information on the Maxwell Centre and the new laboratories and the science taking place in these is described in this report.

Winton Berkeley Exchange Programme

A new Exchange Programme has just been established between the Winton Programme and the Kavli Energy NanoSciences Institute (ENSI) (**kavli.berkeley.edu**) at the University of California, Berkeley to support complementary research between the two programmes. The ENSI brings together researchers across the fields of materials science, physics, engineering, and biology with the aim of improving the performance of existing energy technologies and developing entirely new ways of harnessing energy. The remit is therefore closely aligned with those of the Winton Programme.

The Programme will facilitate the flow of research ideas and promote new activities between the two institutes, through the exchange of researchers in both directions. The first placements are anticipated to take place next year, with support to be provided for the following schemes:

- PhD students
- Postdoctoral researchers
- Faculty members on sabbatical visits

WINTON SCHOLARS 2015/16

Jesse Allardice
Supervisor: Dr Akshay Rao
Optoelectronics Group

"Understanding and controlling ultrafast charge separation at organic and hybrid interfaces"

Alessio Caciagli
Supervisor: Dr Erika Eiser
Optoelectronics Group

"Liquid and gel-droplets moved by light on a surface"

Sean Cormier
Supervisor: Professor Jeremy Baumberg
Nanophotonics Group

"Real-time optical study of structural phase transitions in battery nanoparticles"

Jannes Gladrow
Supervisor: Professor Ulrich Keyser
Biological and Soft Systems Group

"Novel Biomimetic Filtering Concept"

Evelyn Hamilton
Supervisor: Professor Pietro Cicuta
Biological and Soft Systems Group

"Emergence, sustainability and a new approach to motile cilia"

Hannah Laeverenz Schlogelhofer
Supervisor: Dr Ottavio Croze and Professor Alison Smith
Biological and Soft Systems Group and Department of Plant Sciences

"Quantifying Algal-Bacterial Mutualisms"

Lauren McKenzie-Sell
Supervisor: Professor Stafford Withington and Professor Jason Robinson. Quantum Sensors Group and Department of Materials Science and Metallurgy

"Non-equilibrium spin transport in nanostructured Zeeman split superconductors"

Sofia Taylor Coronel
Supervisors: Dr Suchitra Sebastian
Quantum Matter Group

"Search for pressure induced superconductors"

The funding for the Maxwell Centre was obtained as a result of a successful bid to the Higher Education Funding Council's UK Research Partnership Infrastructure Fund (UKRPIF). The Fund provided £21M which was supplemented by £4.6M from the University. The grant was made on the basis that the Laboratory and its partners had generated £42M from non-governmental sources, including the Winton Programme, and this resource provided the operations cost of the science programme. Construction started in July 2014 with the first occupants moving in on schedule in December 2015.

The inauguration of the Centre took place on 7th April 2016, the formal opening of the Building being performed by David Harding. In his remarks he emphasised the collaborative ethos was at the heart of the Centre and how the activities to be carried out were a perfect match to the Winton theme of promoting original, risky and ground-breaking fundamental research.

The Centre is connected to the existing Physics of Medicine building on the West Cambridge site on JJ Thomson Avenue and comprises three floors of offices and a floor for laboratories, housing up to 230 researchers. The total usable space is over 3,000 m² which includes 700 m² of laboratory space, which is enhanced by a further 500 m² of reconfigured areas within the Physics of Medicine building.

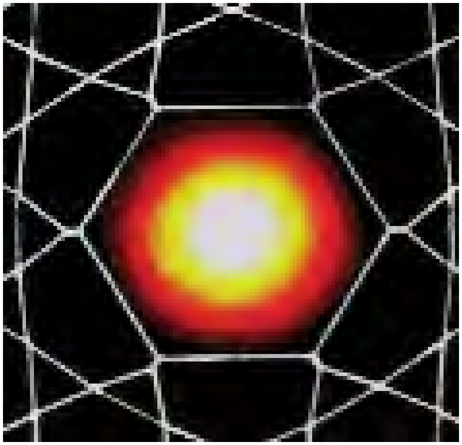
The majority of the Winton Fellows and Winton affiliated Lecturers have moved into the Maxwell Centre; in many cases they have been able to design their new laboratories to meet their specific research requirements. These include the materials fabrications and characterisation suites developed by Lecturers Suchitra Sebastian and Siân Dutton, the opto-fludic micro-reactor laboratory of Lecturer Tijmen Euser and the ultrafast spectroscopy setup of Winton Fellow Akshay Rao. To meet the collaborative aims of the Maxwell Centre many of the laboratories have been designed to enable access to other users. Other laboratories in the Centre will also contribute shared access facilities including those managed by the Centre for Doctoral Training on Nanoscience which has set up a series of tools to characterise materials down to the nanoscale. Equipment will also be housed in the Centre as part of the Cambridge component of the Sir Henry Royce Institute for Advanced Materials. The Maxwell Centre will be home to researchers from across the Physical Sciences; the Materials Department already has a significant presence with their industrial collaboration with SKF, and will be joined by researchers from Chemistry and Engineering and other industrial partners. The student community will also be well represented in the Centre through the Nanoscience and Computational Methods for Materials Science Centres for Doctoral Training (CDTs). Both CDTs perform interdisciplinary research, bringing supervisors and research projects from across the University to the Centre. There is also a strong overlap with the Winton Programme with several students being supervised by Winton Fellows.

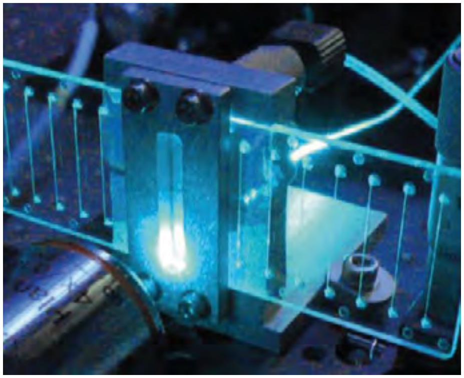
Left: David Harding at the opening of the Maxwell Centre; right: The Maxwell Centre

MAXWELL LABORATORIES

Optofluidics Laboratory, Tijmen Euser Lecturer in Physics and affiliated to Winton

The Maxwell Centre Optofluidics laboratory develops novel optofluidic devices based on liquid-filled hollow-core photonic crystal fibres, fibre tapers, and micro-capillaries. Current research directions include in situ reaction monitoring and optical manipulation of nanoparticles. These studies are expected to have a strong impact on the development of new catalytic and photochemical systems and in the development of novel light-activated anti-cancer drugs. Another important application area is waveguide-based optical characterization and separation of plasmonic- and semiconductor nanoparticles.

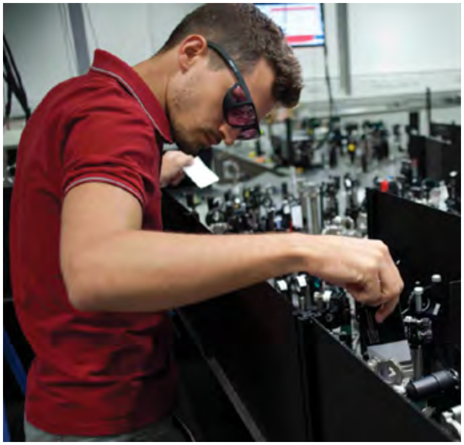




Our laboratory is well-equipped with a range of novel optical techniques, including a high-power broadband supercontinuum source (480-2200 nm), a tuneable CW Ti:Sa laser system (725-975 nm, max output 5 W), various spectrometers, spatial light modulators, and fibre launch systems. We are currently also setting up a post processing setup capable of tapering optical fibres and capillaries. While most of our equipment is integrated into custom-built experimental rigs, we are always happy to discuss possible collaborations in related research fields.

Ultrafast Laboratory, Akshay Rao Winton Advanced Research Fellow

Understanding the flow of charges and energy in matter is of fundamental interest and also the key to building next-generation energy efficient devices. In our newly opened Winton Laser Labs, we are developing a laser spectroscopy system that enables us to measure the electronic and vibrational dynamics of matter on sub-10fs timescales and with sub-diffraction length spatial resolution. This world leading capability will allow us to visualise the dynamical flow of electrons and quasipartricles, such as excitons, on their natural time and length scales. Our techniques also allow us to understand how these excitations couple to phonons and molecular vibrations. We are currently applying these methods to study a range of semiconductor materials, such as organic, hybrid-perovskite, quantum dots and 2D materials.



Quantum Materials Laboratories, Siân Dutton and Suchitra Sebastian University Lecturers affiliated to Winton

The Quantum Materials group was created in 2015, and is based in the new Maxwell Centre in the Department of Physics, University of Cambridge. Our research deals with complex quantum materials. Interactions between trillions and trillions of electrons in these materials lead to new collective quantum behaviour that is dramatically different from the well-understood behaviour of individual electrons. In the Quantum Materials group we seek to discover and understand new quantum phases of matter. Our research techniques involve thermodynamic, transport, and structural measurements of a variety of new materials. We search for exotic quantum behaviour by a combination of novel materials' synthesis, characterisation, and the tuning of materials' properties using extreme conditions including very low temperatures, high magnetic fields, and large applied pressure.

The new laboratories in the Maxwell Centre are fully equipped for materials synthesis, characterisation of thermodynamic, transport, and structural properties, and measurement of physical properties under a broad range of temperatures, magnetic fields, and applied pressure. The Quantum Materials laboratory also manages the multi-user Maxwell Centre powder diffraction X-ray facility, together with the Advanced Materials Characterisation Suite which enable the characterisation of the structural, electrical, magnetic and thermal properties by users from across the University and further afield.

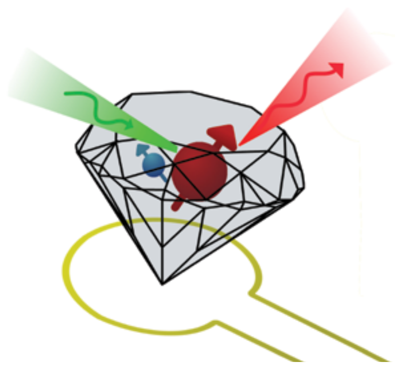
ESPRC/Winton advanced materials characterisation suite: X-ray, magnetic and electrical characterisation tools for complex materials

Fully supported by technical staff, the Advanced Materials Characterisation Suite is designed to accommodate both expert and inexperienced users.

Equipment in the Advanced Materials Characterisation Suite includes equipment for the characterisation of crystal structures (Laue camera), magnetic properties (SQUID Magnetometer), electronic properties (Physical Properties Measurement System) and high field, low temperature electrical and magnetic properties measurements (VERSMAG).

SCHOLARSHIPS

Jan Beitner is working on nanoscale magnetic, electric, and temperature sensing. In particular, he is interested in using the electron spin of the nitrogen-vacancy centre, which is an atomic defect in diamond, for high precision measurements. This quantum sensor can be initialised and read out optically and manipulated with microwaves and therefore does not require electrical connections. Embedded in a nanodiamond, it has potential applications in biology, especially for in vivo sensing in cells. However, the defect's sensitivity in nanodiamond is currently limited due to crystal impurities and its proximity to the surface. This is why Jan explores possibilities to increase its sensitivity by utilizing the nitrogen nuclear spin, intrinsic to the defect. Jan's work contributes to the development of nitrogen-vacancy centres into a standard metrology and materials research tool.



Nitrogen-vacancy centre in nanodiamond

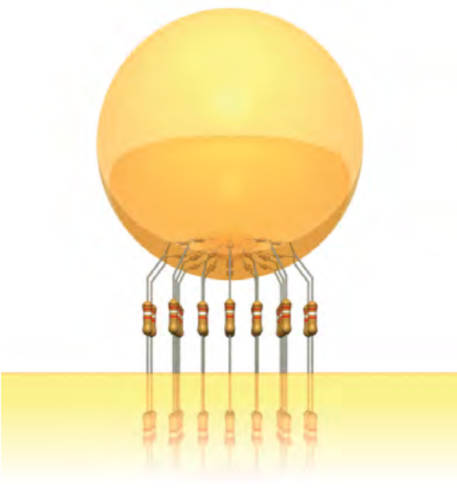


Illustration of a plasmonic gold nanostructure shunted with conductive molecules

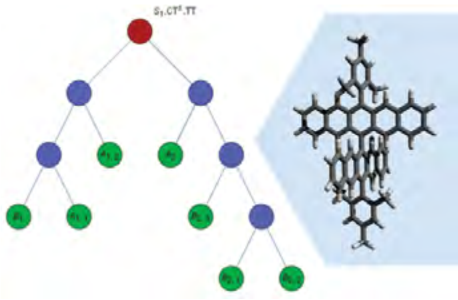
Felix Benz's research is focused on the light-matter interaction of organic molecules in nano-optical fields created by plasmonic gold nanostructures. In these structures coupled localised surface plasmon polaritons are used to confine electromagnetic radiation to volumes of only tens of cubic nanometres, resulting in an enhanced interaction of molecules and light.

One main aspect of Felix's work is the impact of a molecular conductance on these coupled plasmonic modes. Exchanging the insulating molecules for a conductive variant allows charges to be exchanged between the nanoparticle and the gold film. This current alters the nature of the plasmonic modes by screening the charges in the gap region (Nano Letters 15, 669, 2015). This research opens the possibility of exploring new ways to interface optics and electronics on the nanoscale.

Kerstin Göpfrich has been working on DNA origami, the science of folding DNA to sculpt matter at the atomic level. She used DNA to build membrane-inserting synthetic channels. Given that 50 percent of drugs target natural channels in cells, synthetic channels can advance our understanding of the mechanisms of disease and serve as novel therapeutics. Amongst various other architectures, she created the largest man-made pore in a lipid membrane to date. Pushing the boundaries on the other end of the spectrum, her work demonstrated the ultimately smallest DNA

Pore made from DNA attached to a membrane

membrane pore from a single membrane-spanning DNA duplex. Thereby, it was shown that ion-conduction across lipid membranes does not require a physical channel – which Kerstin calls the most exciting insight of her PhD.



Florian Schröder studies excited state dynamics of organic molecules that can be highly correlated with inter- and intramolecular vibrations and therefore exhibit dynamics which cannot be described within the typical Born-Oppenheimer approximation. Including these environmental modes into the model and simulating it is a challenging task. Florian's research focuses on the development of a new tensor network technique based on matrix product states (MPS) (Phys Rev B93, 075105, 2016). Through strong and adaptive compression of the many-body wavefunction it is able to simulate open quantum system dynamics under multiple structured environments.

He applied his method to simulate pentacene dimers and demonstrated that the method allow the comparison of excitonic with vibrational dynamics revealing the mechanisms of singlet fission in this molecule.

His research closes a gap between MPS, originated in theory of condensed matter, and Hartree-Fock techniques from quantum chemistry by combining their respective advantages.

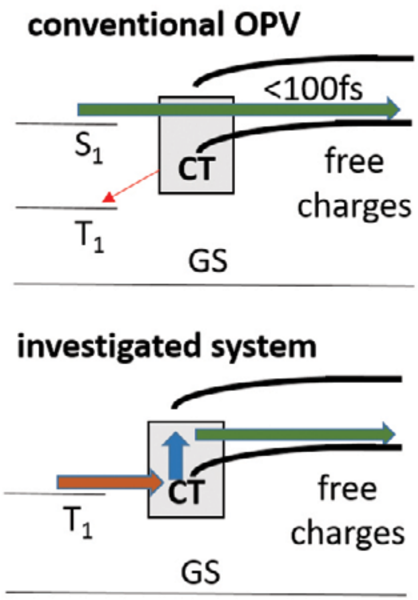
Zachary Ruff's research focuses on how DNA-colloidal self-assembly can be used to form ordered materials with feature sizes of hundreds of nanometers though tuning the interaction potential between colloids. Forming bulk three-dimensional materials at this length-scale remains a challenge for both top-down and self-assembly techniques. Meeting this challenge could enable new functional materials for applications including energy storage and passive displays. He has demonstrated how blue colors can be formed through engineering the structure of DNA-colloidal gels and is currently developing new

Blue pigments made from DNA-NP gels

methods for forming high rate battery electrode materials.

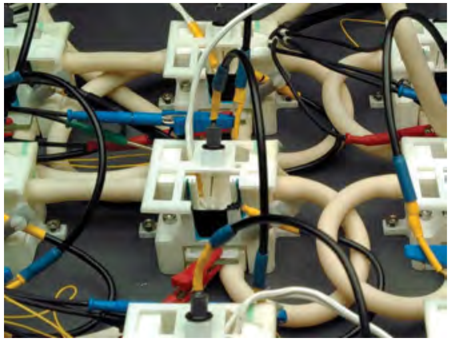
Hajime Shinohara's research focuses on doping effects in geometrically frustrated magnets (GFMs). Frustrated magnets are magnetic materials which have degenerated ground states because of the competing magnetic interactions. In particular, he is interested in the interactions of spins in spin ices, the magnetic analogues of water ice, and one dimensional quantum frustrated magnets. Hajime synthesises and characterises the materials using a ceramics process. He then measures and evaluates magnetic properties using magnetisation and heat capacity measurements. From his research, it is seen that doping in GFMs has a dramatic effect on their properties.

Maxim Tabachnyk has been investigating how much energy must be lost in converting bound excitons to free charges, which is key to determining the achievable open-circuit voltage in excitonic solar cells. In his research, which was supervised by Richard Friend and Akshay Rao, he used ultrafast transient optical spectroscopy to show that excitons can be separated into charges with very low energetic loss. This charge separation against a Coulomb barrier is modelled to be driven by entropy, leading to an effective voltage loss of only 400 meV, comparable to silicon. The results show that an excitonic photoconversion system can separate charges with near unity efficiency while minimising loss of open-circuit voltage, which promises to achieve organic solar cells with power conversion efficiencies of up to 20%.



Comparison of free charge generation in conventional organic photovoltaics (OPV) with high voltage loss and the investigated system with low voltage loss.

Tobias Wenzel integrates living biological organisms into technological sustainable energy solutions in order to utilise their unique abilities to self-replicate, self-repair, and catalyse complex and specific reactions under mild conditions, while being biodegradable. Specifically, he works on photosynthetic bacteria that allow production of electricity directly from sunlight in a self-renewing system. His quantitative measurements of photo-electric activity in model organisms and genetically modified species provided valuable insights into how photosynthetic organisms handle the energy gained from light. He has combined the theoretical framework he has developed to predict quantitatively light-energy utilisation in biofilms with his design of a 3D-printed system for bioelectric measurements. In this way, he has advanced biological photo-electric measurements into a new tractable tool for cell-energetics. Tobias' recent successes in engineering the electrode bio-interface enhanced the quantum efficiency of devices by two orders of magnitude.



3-D printed devices for quantitative and temperature controlled electrochemical measurements of photo-electrons from microorganisms.

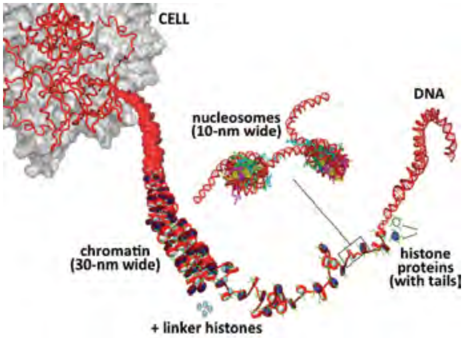
FELLOWSHIP

Rosana Collepardo

My research group investigates the design principles of data storage in chromosomes and chromatin and aims to translate these principles into design rules for novel sustainable data storage devices. Our research also exploits principles from physics, chemistry, computer science, and biology to unravel the relationship between epigenomes, chromatin structure and gene function. Although it is recognized that epigenetic factors play a crucial role in regulating normal and aberrant gene function, the detailed molecular mechanisms that explain these roles and their effects on genomic structure are not clear. Our group investigates these questions by developing and applying novel multiscale computational methods that are anchored in all-atom molecular dynamics simulations, coarse-graining techniques, theory, and experiments from collaborators. Unlike other approaches, our methods can connect subtle chemical changes to broad topological transformations in large biomolecular systems (JACS, 2015 137:10205, PNAS 2014, 111:8061).

During my first six months as a Winton Fellow, I have recruited two PhD students, Sivapalan Chelvaniththilan (Gates and Winton Scholar) and Steve Farr (CDT computational methods), and one MPhil student, Akshay Srindhar (CDT computational methods), that have just started their chromatin work this term, and co-supervised one MPhil student. I have continued working with my collaborators in the Chemistry Department (Profs. Shankar Balasubramanian, Daan Frenkel, David Wales, and Michele Vendruscolo) and New York University (Tamar Schlick), and established two new experimental collaborations with Prof. Peter Fraser (Babraham Institute) and Prof. John van Noort (U of Leiden).

Sivapalan is currently developing a new chromatin coarse-grained model that considers nucleosome unwrapping and incorporates single-molecule force-extension experimental data of chromatin from Prof. van Noort. Using new single-molecule HiC data from Prof. Fraser's lab, Steve will investigate the structure of chromatin inside chromosomes during active and inactive gene transcription stages. Akshay will build a new scientific visualization package to analyse chromatin structure at the nanoscale and refine the Martini force-field for proteins and DNA to reproduce chromatin experimental observables.



Chromatin (our genome at the nanoscale): Inside our cells, the DNA is not found free, it is wound around proteins (histones), forming a remarkable structure know as chromatin. The figure illustrates the hierarchical folding states of nanoscale chromatin showing the DNA in red, alternating nucleosomes in white and blue, and histone tails in green. Through chromatin, the DNA compresses enormously to fit inside tiny (6 μm) nuclei, stores information at high densities and, moreover, maintains exquisite control over the accessibility of the data it carries. Chromatin regulates access to its DNA through an extra layer of information known as epigenome. The epigenome consists of a pattern of chemical modifications of the DNA and histone proteins, unique to each cell type. Epigenomes allow the same DNA sequence to be interpreted differently and generate diversity of functions.

PROGRAMME HIGHLIGHTS

Carbon reduction technologies discussed at World Economic Forum

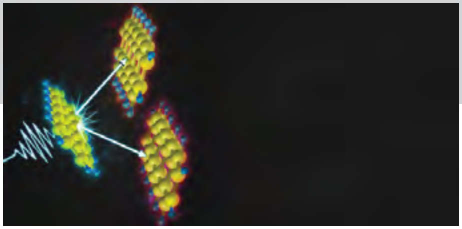
A University of Cambridge delegation of academics attended the World Economic Forum annual meeting in Davos to explore carbon reduction technologies and how science and engineering can best address society's greatest challenges.

Richard Friend explained how it is possible to harvest more power in solar cells by splitting high-energy photons. He also discussed how quantum mechanics could improve the efficiency of solar materials, explaining that there is longer-term potential to develop technologies that can manufacture photovoltaics using less material.

Suchitra Sebastian highlighted the opportunities for transforming the energy landscape by using superconductors that offer zero-loss transmission of electricity. She described the challenge of improving our understanding of these materials which behave as ensembles driven by quantum effects and how this knowledge will enable the design of new materials.

www.weforum.org/agenda/2016/03/how-can-we-make-solar-cells-more-efficient/

www.weforum.org/videos/quantum-materials-for-zero-loss-transmission-of-electricity-suchitra-sebastian



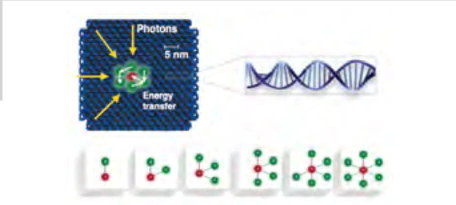
Entanglement at heart of 'two-for-one' fission in next-generation solar cells

A team of scientists including Winton Fellows Alex Chin and Akshay Rao and Winton Scholar Sarah Morgan, have observed how a mysterious quantum phenomenon in organic molecules takes place in real time, which could aid in the development of highly efficient solar cells (Nat Chem, 8, 16, 2016).

Ultrafast laser pulses were used to observe how a single particle of light, or photon, can be converted into two energetically excited particles, known as spin-triplet excitons, through a process called singlet fission. If singlet fission can be controlled, it could enable solar cells to double the amount of electrical current that can be extracted.

A model was developed which showed that when the molecules are vibrating, they possess new quantum states that simultaneously have the properties of both the light-absorbing singlet exciton and the dark triplet pairs. These quantum 'super positions' not only make the triplet pairs visible, they also allow fission to occur directly from the moment light is absorbed.

www.cam.ac.uk/research/news/entanglement-at-heart-of-two-for-one-fission-in-next-generation-solar-cells

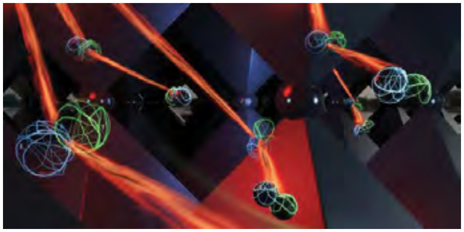


Programming light-harvesting efficiency using DNA origami

The remarkable quantum efficiency of biological light-harvesting complexes has prompted interest in engineering biologically inspired antenna systems as a possible route to novel solar cell technologies. The research groups of Dr Alex Chin, Winton Advanced Research Fellow Professor Ulrich Keyser, Physics Department, with collaborators at TU Braunschweig, Germany and Microsoft Research have demonstrated an artificial, programmable antenna system on a DNA origami platform, enabling them to mimic some of the exquisite nano-engineering of biological light harvesting and explore the optimal co-ordination of pigments.

Creating a library of over 40 assembled antenna structures, they analysed the light-harvesting efficiency with respect to the geometry and number of "donor" pigments (green, in figure) that can capture and transfer photonic energy to an "acceptor" (red) pigment, which is the primary function of photosynthetic antenna complexes. The team was able to predict the efficiency and best geometric arrangement of pigments for this task, which was verified by both ensemble and intricate single-molecule measurement techniques.

http://pubs.acs.org/doi/abs/10.1021/acs.nanolett.5b05139



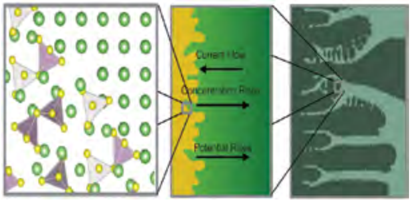
Solar cell material can recycle light to boost efficiency

Scientists have discovered that a highly promising group of materials known as hybrid lead halide perovskites can recycle light – a finding that they believe could lead to large gains in the efficiency of solar cells.

The research led in Cambridge, involved Winton Scholars Monika Szumiło, Johannes Richter and Milan Vrućinić and was reported in the journal Science (351 (6280), 1430 (2016)). The study was undertaken in partnership with the team of Henry Snaith at the University of Oxford and Bruno Ehrler at the FOM Institute, AMOLF, Amsterdam.

Hybrid lead halide perovskites are a particular group of synthetic materials which have been the subject of intensive scientific research, as they appear to promise a revolution in the field of solar energy. As well as being cheap and easy to produce, perovskite solar cells have, in the space of a few years, become almost as energy-efficient as silicon – the material currently used in most household solar panels.

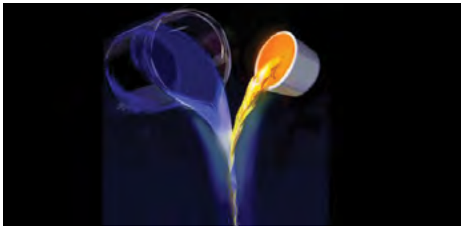
www.cam.ac.uk/research/news/solar-cell-material-can-recycle-light-to-boost-efficiency



Next Generation Solid-State Batteries

A group of collaborators including Winton Fellow Andrew Morris, has secured an Engineering and Physical Sciences Research Council (EPSRC) grant of £2.1 M for a 3-year project to improve the performance of solid-state batteries. The research will combine experimental and computational activities and will be led by Professor Clare Grey, Department of Chemistry, University of Cambridge and involves collaborators at Imperial College London and University of Oxford as well as industrial partners.

Solid-state Li-ion batteries (SSLBs) represent the ultimate in battery safety, eliminating the flammable organic electrolyte. The SSLB would find potential uses in industries where battery safety is paramount, such as the automotive industry (in cars, e-bikes and buses) and also in smaller applications where the elimination of the liquid electrolyte results in more ready compatibility with other devices. Overall, the project aims to provide new strategies to improve the performance of these batteries and also lead to new electrolyte designs that are suitable for protecting Li metal in other so-called "beyond Li-ion" batteries such as Li-air and Li-S.



Nano 'hall of mirrors' causes molecules to mix with light

Researchers in Cambridge, including Winton Scholar Felix Benz, have successfully used quantum states to mix a molecule with light at room temperature, which will aid the exploration of quantum technologies and provide new ways to manipulate the physical and chemical properties of matter.

To use single molecules in this way, the researchers had to construct reliably cavities only a billionth of a metre (one nanometre) across in order to trap light. They used the tiny gap between a gold nanoparticle and a mirror, and placed a coloured dye molecule inside. "It's like a hall of mirrors for a molecule, only spaced a hundred thousand times thinner than a human hair," said Professor Jeremy Baumberg of the NanoPhotonics Centre at Cambridge's Cavendish Laboratory, who led the research (Nature, 535, 127, (2016)).

When assembled together correctly, the molecule scattering spectrum splits into two separated quantum states which is the signature of this 'mixing'. This spacing in colour corresponds to photons taking less than a trillionth of a second to come back to the molecule.

www.cam.ac.uk/research/news/nano-hall-of-mirrors-causes-molecules-to-mix-with-light

NEXT GENERATION BATTERIES

The demand for batteries is increasing rapidly as we move to renewable sources of energy and to power our plethora of mobile devices. It turned out that there is significant headroom for improvement in performance. By understanding the fundamental material science through experiment (Winton affiliated Lecturer Siân Dutton) and theory (Winton Fellow Andrew Morris) new approaches and technologies are being evaluated that could have a significant impact.

It is difficult to overstate the transformative technological role of the lithium-ion battery (LIB), which has the highest capacity of all the commercially available rechargeable battery technologies and is deployed in hybrid and all-electric vehicles, laptop computers and mobile phones. There is huge technological demand for new battery technologies and materials with increased capacity, lifetimes, safety, reduced charging rates and manufacturing costs.

A battery consists of an anode – graphite in most commercialised cells –a cathode - usually a transition metal oxide – separated by the ionically conducting yet electrically insulating electrolyte. There is plenty of scope for new battery materials, for example, silicon has ten times the capacity of the ubiquitous graphite anode, but suffers from a 400% volume change when charged, and Na^+ and Mg^{2+} are far cheaper charge carriers than Li^+ but are less mobile. Should this problem be overcome then they offer high capacity, low cost alternatives to LIBs.

Quantum mechanical modelling is a way to scan for new materials and overcomes many of the challenges associated with experimental investigations. Computational modelling can characterise a material and indicate whether it is worth the effort of finding an experimental synthesis path. This is especially useful with flammable (Li, S), irritant (Mo), toxic (Mn,Ni) or expensive (Au) atomic elements.

Phosphorus has received recent attention in the context of high-capacity and high-rate anodes for lithium- and sodium-ion batteries. Martin Mayo, Andrew Morris along with co-workers in the Department of Chemistry have presented a computational structure prediction study combined with NMR (nuclear magnetic resonance) calculations, which gives insights into its lithiation/sodiation process. They have reported a variety of new phases of Na- and Li-P suggesting that black phosphorus can be considered as a safe anode in lithium-ion batteries due to its high lithium insertion voltage; moreover, black phosphorus exhibits a relatively low theoretical volume expansion compared with other intercalation anodes, 216% ($\Delta V/V$).

In another recent study Morris in collaboration with Dr Michael De Volder's group at the Institute of Manufacturing, has combined calculations with electrochemical synthesis on molybdenum disulfide (MoS_2). MoS_2 offers a capacity up to 3-times higher (~1 Ah/g) than the currently used graphite anodes, but it suffers from limited efficiency and capacity fading. They found new sulfur-enriched intermediates that progressively insulate MoS_2 electrodes and cause instability from the first discharge cycle. Because of this, the choice of additives that aid electrical conduction is critical for the battery performance. They investigate the mechanistic role of carbon additives by comparing equal loading of the standard carbon powder binder and carbon nanotubes (CNTs). The latter offer a nearly 2-fold increase in capacity and a 45% reduction in resistance along with efficiency of over 90%. These insights into the phase changes during MoS_2 conversion reactions and stabilization methods provide new solutions for implementing cost-effective metal sulfide electrodes, including Li–S systems in high energy-density batteries.

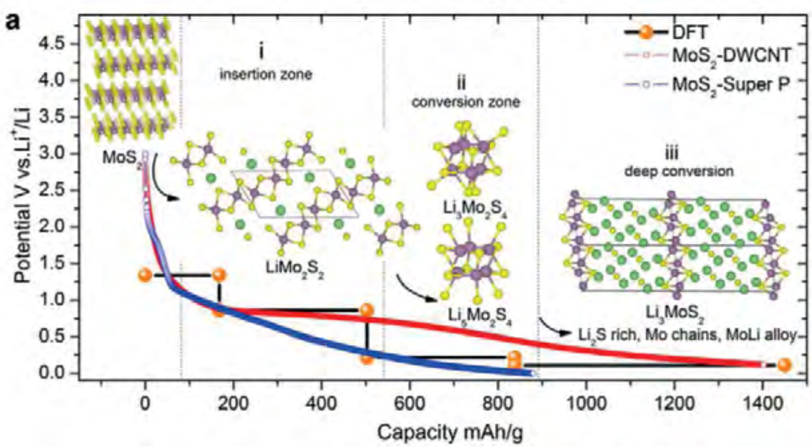


Figure 1: Representative discharge profiles from the first cycle of MoS_2^+ double-walled carbon nanotubes (DWCNT) and MoS_2-Super P electrodes together with the average voltages calculated from theory (DFT) energies, relative to Li^+/Li and assuming each reaction is 2-phase: (i) For the metastable $LiMo_2S_2$ phase, the sheets are buckled. (ii) For MoS_2, 2 clusters found in a sea of Li, the clusters $Li_3Mo_2S_4$ and $Li_5Mo_2S_4$ are found, with the sulfur being pulled away from Mo and toward the Li. (iii) The Li_3MoS_2 phase leading to segregated Li_2S regions.

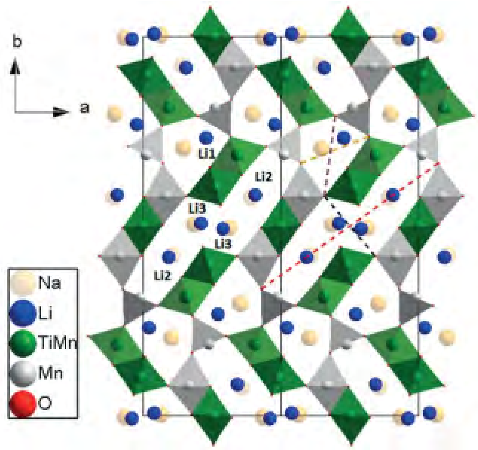


Figure 2. Polyhedral representation of the crystal structure of $LiMnTiO_4$ viewed down the c axis. The original Na sites are also shown.

A recent study in the Dutton group has explored the electrochemical properties of kinetically stablised materials. Prepared using soft methods these types of materials are difficult to predict and model theoretically and so only experiments provide new insight. They studied the properties of a Mn-Ti-oxide with an open structure, and find that there is rapid Li-ion transport of one equivalent Li-ion. Their results on iron containing analogues also show promise as electrodes for Li-ion batteries. The team, together with collaborators in the Chemistry department, are now using similar routes to investigate materials for Mg-ion batteries. This will allow a systematic study on the Mg-ion transport which at present restricts Mg-ion transport in high voltage systems.

More info from

Structural Evolution of Electrochemically Lithiated MoS2 Nanosheets and the Role of Carbon Additive in Li-Ion Batteries, *Chandramohan George, Andrew J. Morris, Mohammad H. Modarres, and Michael De Volder*, Chem. Mater. *As Soon as Publishable* (2016), DOI:10.1021/acs.chemmater.6b02607

Ab Initio Study of Phosphorus Anodes for Lithium- and Sodium-Ion Batteries, *M. Mayo, K. J. Griffith, C. J. Pickard and A. J. Morris*, Chem. Mater. **28** 2011-2021 (2016), DOI:10.1021/acs.chemmater.5b04208

$LiMnTiO_4$ with the $Na_{0.44}MnO_2$ Structure as a Positive Electrode for Lithium-Ion Batteries *A. M. Amigues, H. F. J. Glass and S. E. Dutton J. Electrochem. Soc.* ***163*** *A396-A400* (2016) DOI: 10.1149/2.0231603jes

www.andrewjmorris.org

PUMP PRIMING

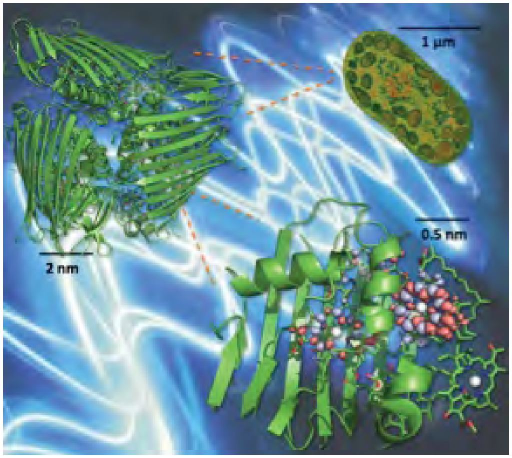
The Pump Prime scheme provides funding of up to £50k to researchers in the Department and collaborators from other departments for new research activities. The scheme aims to fund innovative high-risk activities, rather than on-going research, that if successful could have significant impact. Some recent grants are described here with further information including how to apply on the Winton website at www.winton.phy.cam.ac.uk/pumpprime

Quantum mechanical modelling of energy transport in photosynthetic pigment-protein complexes

Dr Alex Chin and Dr Tim Zuehlsdorff (TCM), Dr Daniel Cole (Newcastle University) and Dr Nicholas Hine (University of Warwick)

The high efficiency of photosynthetic light reactions has been studied for many decades, revealing the critical role of optimised, purpose-built biological nanostructures, known as pigment-protein complexes (PPCs), in directing solar energy transport. The underlying physics of this versatile class of "devices" are still not fully understood, yet the recent and unexpected discovery that PPCs can support robust quantum ("wave-like") dynamics has brought forth the exciting idea that the answers may lie within a full quantum mechanical theory of PPCs.

This project aims to develop the computational tools to provide such a description, enabling us to pinpoint the role of quantum effects in natural PPCs and also how such normally fragile effects are shielded from the noisy biological environment. Using new advances in linear-scaling quantum mechanical simulations we will provide novel insight into the hierarchy and interconnections between structure, electronic properties and functional dynamics which are uniquely exploited in PPCs.



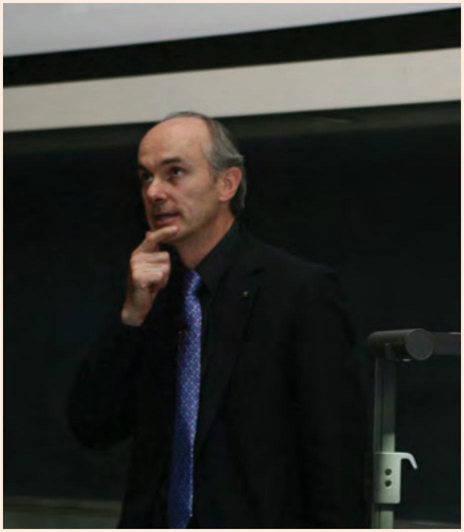
Structural similarity algorithms for novel materials discovery

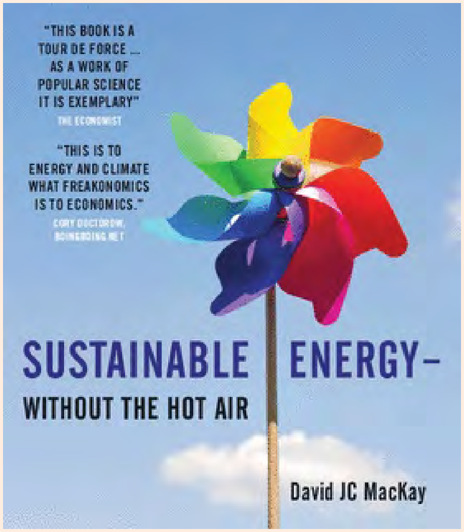
Dr Andrew Morris (TCM) and Dr Matthew Dunstan and Professor Clare Grey (Department of Chemistry)

We are at the threshold of a Big Data revolution, and with the advent of large libraries of either experimentally or theoretically determined structures of crystalline solid state materials that are easily accessible, there is an opportunity to adapt the techniques used in organic chemistry and structural biology to crystalline, close-packed materials.

This interdisciplinary project will develop new computational tools designed to extract new insights into the design of advanced functional materials from structural databases. One of the aims is to develop an algorithm that is able to screen thousands of materials for their predicted oxygen ionic conductivity to discover new candidates for solid oxide fuel cells.

DAVID MACKAY
1967–2016





Sir David MacKay, who died of cancer aged 48, was a pioneering scientist as well as a tremendous teacher and role model. His early research on computation and neural networks led to the establishment of the Inference Group at the Cavendish with his book on Information Theory, Inference and Learning Algorithms (2003 – free to download at **www.inference.phy.cam.ac.uk/itila**) becoming a standard text for many students and was the basis for the development of Bayesian methods and other related topics such as Machine Learning which are having an impact in a large range of fields.

In the context of the Winton Programme his book 'Sustainable Energy – Without the Hot Air' (2008 – free to download at **www.withouthotair.com**) became an essential read for anyone interested in understanding the energy challenges we face. The book provides a lucid analysis of our energy consumption and generation options which is based on 'numbers, not adjectives'.

His appointment in 2009, as Chief Scientific Advisor to the Department of Energy and Climate Change (DECC) was timely with David able to convey his quantitative approach to this pressing global problem. One of his major achievements during his tenure was the development of the interactive online 2050 calculator. This enabled non-experts to evaluate the consequences of different strategies for meeting the UK's target to reduce its carbon emission by 80% by 2050. The tool helped people have informed conversations to move the debate forward and attracted considerable international interest, with many countries developing their own calculators.

The work was expanded by David and colleagues at DECC to produce a calculator to evaluate the global temperature rise as a consequence of adopting different strategies. This 'Global Calculator' was the topic for his talk at the Winton Symposium in 2014 on Global Challenges, where he explained that to stop any further climate change the CO_2 emission rate needs not only to decrease but to drop to zero. To achieve this not only do we need to reduce emissions but negative emission technologies have to become available on a global scale.

David was an International Advisory Board member for the Winton Programme and instrumental in establishing the Winton teatime discussions. These informal gatherings enabled students and others from the Department and outside to debate a topical issue, with David providing his insight on scientific solutions as well as practical actions.

WINTON EVENTS

Winton Symposium on Green Computing

The 4th Winton Symposium was held at the Cavendish Laboratory on 28th September 2015, on the topic of Green Computing. This is a field where there is considerable scope for advances in basic science to impact our energy consumption. Through more energy efficient devices and systems, as well as the increasing computing power being used to do things more efficiently.

Mike Lynch, founder of Invoke Capital and Autonomy, explained how the power and cooling needs of data centres has become a major operating cost. This has led to the development of new architectures with 'hot' and 'cold' servers. Also instead of focusing solely on moving energy to where the processing takes place, taking data to the source of power is also becoming a viable proposition. The increase in the amount of computation power and data from the proliferation of sensors will markedly improve pattern recognition. This will impact on a host of activities, from crop growth to route guidance systems, providing sustainable benefits from the additional computing capability.

Andy Hopper, Head of the Computer Laboratory at the University of Cambridge, in his talk, 'Computing for the Future of the Planet', considered what we can do better with computing and how this can have societal benefits. He described the increase in efficiency of digital infrastructure that had led to stabilisation of the total energy consumption, and how the availability of sensors and data can be used to do things more efficiently. Computing can lead to an overall energy gain as long as the assurance and governance are set up right and with the benefits able to reach out to everybody on the planet

Krisztián Flautner, head of ARM's Internet of Things (IoT) Business Unit, explained how IoT was based on the convergence of devices, computing and connectivity. With sensors and microprocessors available so cheaply the time is right for numerous opportunities with a strong business case. For this emerging field the metrics for evaluation will need to evolve, whereas for mobile communication the key parameters were performance, energy and price, trust and scale have to be included. IoT will generate vast quantities of data, which will only be trusted if ownership, access and privacy issues have been resolved. This will require control of the data and establishment of standards across the globe. IoT will require many different partners to work together to make the number of products needed that connect together; an ecosystem is being built that encompasses all aspects from hardware to the cloud that will enable people to build the appropriate IoT solutions.

Luca Cardelli, from Microsoft Research and University of Oxford, in his talk 'Molecular Programming' introduced a totally different way of doing computing using biological materials. From a hardware perspective traditional computing has been making components smaller and smaller; instead if we start with molecules or DNA the problem becomes how can we build systems. In nature this bottom-up approach is routinely achieved through using self-assembly with materials pre-programmed to fit to each other. Although the field is still in its infancy and it will take some time to find practical solutions, it is growing rapidly and the promise is amazing.

Linda Nazar, from the University of Waterloo, discussed the recent development of batteries and explained that storage is more important today than ever before, with integrated systems required to meet our growing demand for large and small scales of energy. For grid storage more abundant materials are being considered, including using Na instead of Li, as well as divalent ions where weight is less of an issue. Another important area is the exploration of solid state electrolytes, which have a number of benefits including being less hazardous, easier to package and make into thin films and prone to longer cycle life. Battery chemistry is complex and involves not just the electrodes but also the electrolyte and interfaces, an improved understanding will spur on progress on finding different solutions for different energy storage applications.

Hideo Ohno, from Tohoku University described how very large-scale integrated (VLSI) circuits are prevalent in so many aspects of our lives. Power consumption has grown as devices become more complex with more active components, but an equally important factor is the increase in the standby power due to higher leakage currents. Another challenge is that of interconnection delay, associated with systems having separate logic and memory components and information needing to be passed between the two, which causes delay and consumes power. One solution is to move from volatile memory to non-volatile memory which reduces considerably the standby current losses. By placing memory on top of the logic plane it is possible to integrate the devices to reduce the interconnection delay. He also proposed a new paradigm in VLSI where circuit designers and process engineers would work together to integrate spintronic logic and memory which will provide solutions that are both greener and have higher performance.

Winton Meeting on Caloric Materials

Magnetocaloric, electrocaloric and mechanocaloric effects are reversible thermal changes that are currently studied near phase transitions in magnetically, electrically and mechanically responsive materials due to changes in magnetic, electric and mechanical field. These materials are suggested as replacements for the harmful fluids used in refrigeration and air-conditioning. It is therefore important to improve their heat-pump performance in terms of temperature span, cooling power, and energy efficiency.

The Winton Meeting on Caloric Materials took place in Cambridge on 10-11 February 2016. The organisers Dr Xavier Moya, Dr Sohini Kar-Narayan and Professor Neil Mathur form the Department of Materials Science and Metallurgy brought together over 50 scientists and engineers from 18 countries. The meeting covered all the types of caloric materials, and ranged from fundamental aspects to applications.

The proceedings of the meeting were published in *APL Materials*, volume 4, issue 6, in June 2016. As an open access publication, the articles in the proceedings are freely available to read, download, and share without a subscription.

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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

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Opposite page, top left to bottom right:

Jan Mertens, Sarah Morgan, Michael Price, Milan Vrucinic, Hannah Stern, Dr Andrew Ferguson, Steffen Illig, Jan Beitner, Monika Szumiło, Vahe Tshitoyan, Di Jin, Bhaskaran Nair, Gabriel Constantinescu, Dr Anoop Dhoot, Dr Tijmen Euser, Jerome Burelbach, Johannes Richter, Sam Schott, Dr Amalio Fernández-Pacheco, Dr Andreas Nunnenkamp, Yago Del Valle-Inclan Redondo, Leah Weiss, Dr Akshay Rao, Professor Neil Mathur, Paromita Mukherjee, Xiaoyuan Sheng, Dr Nalin Patel, Professor Sir Richard Friend, Professor Ulrich Keyser, Professor Jeremy Baumberg, Martin Mayo, Kerstin Göpfrich, Dr Andrew Morris, Professor Ullrich Steiner, Professor Henning Sirringhaus, Dr Nicholas Hine, Dr Siân Dutton, Zachary Ruff, Dr Ottavio Croze, Maxim Tabachnyk, Wenting Guo, Dr Alex Chin, Feliz Benz, Adrien Amigues, Dr Erika Eiser, Tobias Wenzel, Sam Smith, Andreas Jakowetz, Professor Christopher Howe, Dr Suchitra Sebastian, Florian Schröder, Hajime Shinohara, Professor Clare Grey, Professor Mete Atatüre, David Turban, Dr Felix Deschler, Alessio Caciagli, Lauren McKenzie-Sell, Dr Rosana Collepardo, Jesse Allardice, Profoessor Pietro Cicuta, Dr Sarah Bohndiek, Alex Welbourne, Evelyn Hamilton, Dr Chiara Ciccarelli, Dedalo Sanz Hernaandez, Dr Hannah Joyce, Sean Cormier, Hannah Laeverenz Schlogelhofer, Jannes Gladrow, Sofia Taylor, Ture Hinrichsen

THE WINTON PROGRAMME FOR THE

Physics of Sustainability

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