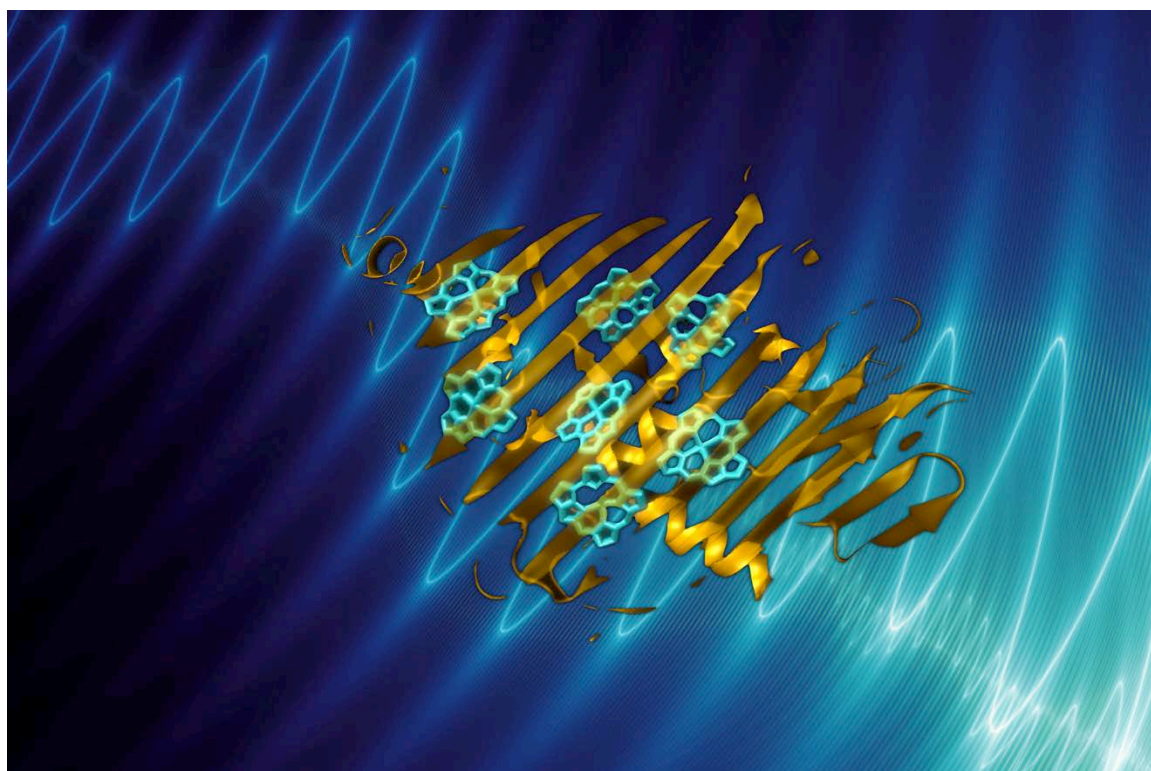


NEW FRONTIERS FOR QUANTUM TECHNOLOGY IN BIOLOGICAL AND BIO-INSPIRED SYSTEMS

Robinson College, University of Cambridge

Umney Theatre, Grange Road,
Cambridge CB3 9AN, UK

18th-19th March 2015



Wednesday 18th March 2015

Introduction	
0930-1000	Coffee and registration
1000-1030	Professor Johnjoe McFadden & Professor Jim Al-Khalili (University of Surrey) The prehistory of quantum biology
Session I	
Quantum Effects in Photosynthesis: Evidence, Theory and Future Directions	
Chair	Professor Richard Cogdell (University of Glasgow)
1030-1115	Professor Gregory S. Engel (University of Chicago) Extracting lessons from Quantum Biology: Probing design principles of energy transfer photosynthetic systems
1115-1200	Dr Alexandra Olaya-Castro (University College London) Non-classical phenomena in photo-activated biomolecules
1200-1330	Lunch and poster session
Session II	
The Machinery of Photosynthesis: From Ultrafast Quantum Dynamics to Water Splitting	
Chair	Professor Tõnu Pullerits (Lund University)
1330-1415	Professor Rienk van Grondelle (VU Amsterdam) The Quantum design of Photosynthesis
1415-1500	Dr Erwin Reisner (University of Cambridge) Photoelectrochemistry of the Water Oxidation Enzyme Photosystem II
1500-1530	Coffee Break
Session III	
New Frontiers for Coherence in Organic Systems: Towards Quantum Technology	
Chair	Dr Alex Chin (University of Cambridge)
1530-1615	Professor Sir Richard Friend (University of Cambridge) Photogenerated excitons and charges in molecular semiconductor photovoltaic devices
1615-1700	Professor Niek van Hulst (ICFO, Barcelona) Light harvesting complexes, single molecules and coherences
1700-1745	Professor Martin Plenio (Ulm University) Quantum Technologies and Biology
1830-1900	Drinks Reception – Balcony of dining hall, Robinson College
1900-	Workshop dinner & speech by Professor Sir Peter Knight

Thursday 19th March 2015

Session I	Catalysis, Tunnelling and the Dynamics of Single Molecules
Chair	Professor Johnjoe McFadden (University of Surrey)
0900-0945	Dr Sam Hay (University of Manchester) H-tunnelling during enzyme-catalysed reactions
0945-1030	Professor Vlatko Vedral (University of Oxford) Probes of quantum behaviour in organic molecules
1030-1100	Coffee Break
Session II	Theoretical modelling of biological nanostructures: from first principles to phenomena
Chair	Dr Ahsan Nazir (University of Manchester)
1100-1145	Dr Nicholas Hine (University of Warwick) Linear-Scaling Electronic Structure Calculations applied to understanding Quantum Effects in biological systems
1145-1230	Professor Susana Huelga (Ulm University) Quantum delocalisation directs antenna absorption to photosynthetic reaction centres
1230-1330	Lunch
Session III	Quantum Sensing in the Natural World
Chair	Dr Erik Gauger (Heriot-Watt University)
1330-1415	Dr Luca Turin (Ulm University) Electron spin changes during general anaesthesia
1415-1500	Professor Henrik Mouritsen (University of Oldenburg) The effects of anthropogenic electromagnetic noise on the magnetic compass of birds and its mechanistic consequences
Session IV	Open Q & A and Panel Discussion
1500-1545	Chair, Panel & Topics TBA
1545-1600	Closing Remarks

Discussion workshop on NEW FRONTIERS FOR QUANTUM TECHNOLOGY IN BIOLOGICAL AND BIO-INSPIRED SYSTEMS

Organised by Dr Alex Chin (University of Cambridge), Professor Johnjoe McFadden (University of Surrey), Elisabeth Wallace (UK Science and Innovation Network)

**Wednesday 18th – Thursday 19th March 2015
Robinson College, University of Cambridge**

Since its modern revival in 2007, the field of Quantum Effects in Biological Systems (QuEBS) has rapidly developed into a high profile interdisciplinary area of physical science, bringing together physicists, chemists and biologists to understand and explore the impact of quantum mechanics in some of the most important biological processes found in Nature. Inspired by the new insights provided by QuEBS, the scope of inquiry is now expanding beyond the still unanswered questions of how and why quantum effects are protected in biomolecular structures. This two-day workshop will investigate one of these exciting new questions; **can QuEBS-like phenomena be artificially engineered for future (quantum) technologies?**

The molecular architectures under study in QuEBS, and particularly those found in photosynthesis, are highly sophisticated, evolved solutions to a range of (biological) problems, and are exquisite examples of nanoscale engineering. While the possible role of quantum mechanics in enhancing efficiencies or robustness in these biological "devices" remains under debate, it is clear that any quantum enhancements operate in a fundamentally different mode compared to other quantum devices, such as quantum computers. Thus, from light harvesting in photosynthesis to avian navigation, natural phenomena provide conceptually new contexts to investigate how quantum effects can be protected and engineered for purpose. As many of the biological problems successfully tackled by Nature are also challenges faced by a range of current technologies, such as organic solar cells, catalysis and sensing, there is a growing opportunity to exploit the developing understanding of QuEBS outside of the biological domain. This potential has been recognized here in the UK, and we are delighted to acknowledge the support of the **UK Science and Innovation Network** in funding this workshop.

This meeting aims to bring together leading researchers in the area of QuEBS and related fields, hoping to facilitate a fruitful exchange of ideas, tools and expertise that may shape the possible development of bio-inspired quantum technologies and further our understanding of quantum effects in biological structure. By presenting the current state of knowledge in QuEBS, its experimental underpinnings, theoretical framework and major questions, we hope to show how developments in this area impact other disciplines, how it could breed novel types of bio-hybrid devices and also how *other* quantum technologies could provide valuable and detailed new information in this area.

Programme and Abstracts

Wednesday 18th March

9:30 Registration

10:00 Introduction

The prehistory of quantum biology

Professor Johnjoe McFadden & Professor Jim Al-Khalili, University of Surrey

In this talk we will discuss how the idea of quantum biology might be involved in biology emerged in the early 20th century with the quantum pioneers who looked for evidence of new physics in biology. One of the group, Pascal Jordan, claimed that living cells were, rather like a dictatorial state, governed by the action of the few (individual molecules) and thereby governed by quantum mechanics. This movement reached its peak with the publication of 'What is Life' by Erwin Schrödinger in 1944 who argued that heredity is based on quantum mechanics, but interest in these ideas declined with the rise of molecular biology. We will examine whether the concepts of these quantum pioneers have relevance to modern quantum biology.

SESSION I: Quantum Effects in Photosynthesis: Evidence, Theory and Future Directions

Session Chair: Professor Richard Cogdell, University of Glasgow

10:30 **Extracting lessons from Quantum Biology: Probing design principles of energy transfer photosynthetic systems**

Professor Gregory S. Engel, University of Chicago

Studies of quantum biology reveal exciting new opportunities to understand robust energy transfer through disordered organic systems. Photosynthetic antenna complexes operate with near perfect quantum efficiency and steer excitonic motion with exquisite precision. These complexes exploit both incoherent (Förster) energy transfer along with coherent (wavelike) motion of energy. My group develops new approaches to isolate and copy the microscopic details of this process. We are particularly interested in how the electronic excitation couples to local vibrations and how these vibrations can steer electronic dynamics. To this end, we build new spectroscopies, theoretical models, and model systems to test our ideas. In this seminar, I will discuss signatures of long-lived electronic coherence, how we measure dephasing rates that determine dynamics, and how we can engineer these effects into synthetic molecular systems. To put these results in context, I will discuss a series of femtosecond spectroscopic measurements on photosynthetic complexes. Next, I will demonstrate *in vivo* 2D electronic spectroscopy, showing energy transfer dynamics in living cells match those in isolated complexes. Finally, I will show novel spectroscopic probes that are providing new windows into dynamics of energy transfer.

11:15 Non-classical phenomena in photo-activated biomolecules

Dr Alexandra Olaya-Castro, University College London

It is well known that primary steps in photosynthesis rely on quantum mechanical phenomena. For instance, excitons or the collective electronic excitations of pigment-protein complexes are a clear manifestation of collective quantum behaviour and they are essential for efficient absorption of sunlight by photosynthetic systems. However, when it refers to excitation energy distribution and conversion in the picosecond time scale, it is not entirely clear which dynamical features can only be predicted within a quantum mechanical framework and how they correlate to the effective energy management by photosynthetic complexes. In this talk, I will review our research on the quest of non-trivial quantum phenomena in photosynthetic complexes with a focus on the emergence and implications of both electronic quantum correlations and non-classical vibrational motion in light-activated molecular systems.

12:00 Lunch and poster session

SESSION II: The Machinery of Photosynthesis: From Ultrafast Quantum Dynamics to Water Splitting

Session Chair: Professor Tõnu Pullerits, Lund University

13:30 The Quantum design of Photosynthesis

Professor Rienk van Grondelle, VU Amsterdam

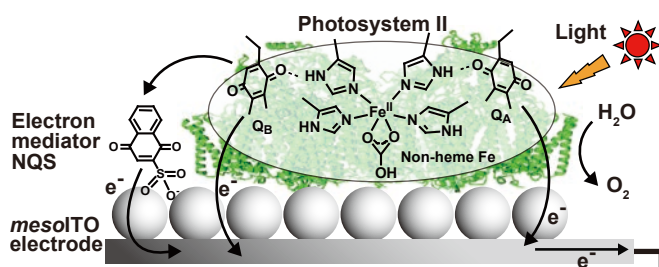
Photosynthesis has found an ultrafast and highly efficient way of converting the energy of the sun into electrochemical energy. The solar energy is collected by Light-Harvesting complexes (LHC) and then transferred to the Reaction Center (RC) where the excitation energy is converted into a charge-separated state with almost 100% efficiency. That separation of charges creates an electrochemical gradient across the photosynthetic membrane that ultimately powers the photosynthetic organism. The understanding of the molecular mechanisms of light harvesting and charge separation will provide a template for the design of efficient artificial solar energy conversion systems.

Upon excitation of the photosynthetic system the energy is delocalized over several cofactors creating collective excited states (excitons) that provide efficient and ultrafast paths for energy transfer using the principles of quantum mechanics. In the reaction center the excitons become mixed with charge transfer (CT) character (exciton-CT states), which provide ultrafast channels for charge transfer. However, both the LHC and the RC have to cope with a counter effect: disorder. The slow protein motions (static disorder) produce slightly different conformations that, in turn, modulate the energy of the exciton-CT states. In this scenario, in some of the LHC/RC complexes within the sample ensemble the energy could be trapped in some unproductive states leading to unacceptable energy losses.

Here I will show that LHCs and RCs have found a unique solution for overcoming this barrier: they use the principles of quantum mechanics to probe many possible pathways at the same time and to select the most efficient one that fits their realization of the disorder. They use electronic coherence for ultrafast energy and electron transfer and have selected specific vibrations to sustain those coherences. In this way photosynthetic energy transfer and charge separation have achieved their amazing efficiency. At the same time these same interactions are used to photoprotect the system against unwanted byproducts of light harvesting and charge separation at high light intensities.

14:15 **Photoelectrochemistry of the Water Oxidation Enzyme Photosystem II**
Dr Erwin Reisner, University of Cambridge

Protein film photoelectrochemistry (PF-PEC) allows for the light-dependent activity of Photosystem II (PSII) adsorbed onto an electrode surface to be studied.¹ We have recently made progress in the direct integration of PSII in conducting metal oxide electrodes. PSII from *Thermosynechococcus elongatus* was adsorbed on a nanostructured and transparent indium-tin oxide (ITO) electrode for visible light driven water oxidation to O₂ and non-mediated electron transfer was observed at the enzyme-electrode interface (Figure 1).² A rational strategy to electrostatically orient and covalently immobilise PSII on the ITO electrode was also developed, resulting in enhanced photocurrent response and film stability.³ In these studies, PF-PEC was shown to provide us with valuable insights into the activity, stability, quantum yields, and interfacial electron transfer pathways of PSII.



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15:00 Coffee Break

Session III: New Frontiers for Coherence in Organic Systems: Towards Quantum Technology

Session Chair: Dr Alex Chin, University of Cambridge

15:30 Photogenerated excitons and charges in molecular semiconductor photovoltaic devices

Professor Sir Richard Friend, University of Cambridge

Organic photovoltaic diodes require a donor-acceptor heterojunction that can split a photogenerated exciton to an electron-hole pair. We have recently found that it is possible to measure the Coulomb energy set up as the electron-hole pair separate, through the modulation of the ground-state optical absorption of the donor caused by the local electric field set up between the electron and hole. We find a substantial electron-hole separation at very early times, setting up an electrostatic field energy of up to 200 meV in times as short as 40 fsecs. This substantial Coulomb energy requires that the electron and hole have fully separated, to at least 4 nm at the very earliest times, and we consider that this arises through direct electron transfer from donor to acceptor states that are delocalised over many acceptor molecules, over distances of 4 nm or more.

Large spin exchange energies allow scope for multiple exciton generation for materials for which the triplet exciton energy is less than one half of the singlet exciton energy, since this favours energetically the fission of a photogenerated singlet to a pair of triplet excitons. If this process can be used in tandem with a lower energy gap semiconductor that harvests singlet excitons directly then this may enhance solar energy conversion beyond the single-junction Shockley-Queisser limit. The Cambridge group has found that this can be achieved using a pentacene/lead selenide hybrid solar cell device structure, for which both triplet exciton and charge transfer can proceed efficiently.

16:15 Light harvesting complexes, single molecules and coherences

Professor Niek van Hulst, Institute of Photonics Sciences, Barcelona

Nature has developed photosynthesis to power life. Surprisingly, quantum coherences are observed in the energy transfer of photosynthetic complexes, even at room temperature. Does nature exploit quantum concepts? Does the coherence help to find an optimal path for robust or efficient transfer? How are the coherences sustained? What is their spatial extent in a real light-harvesting network?

Specializing on femto-nano toolboxes I aim to look ultrafast into the nanoscale, to see molecules in action. Recently we succeeded in the first detection of coherent oscillations of a single photo-synthetic complex at physiological conditions¹, and non-classical photon emission of individual complexes². These results, pave the way to address photosynthetic networks in real nano-space and on femtosecond timescale. Specific

objectives are: *Ultrafast single protein detection*: tracing the fs coherent energy transfer path of an individual complex; addressing the very nature of the persistent coherences. *Detection beyond fluorescence*: light harvesting complex are designed for light transport, not emission. To this end we explore innovative alternatives: optical antennas to enhance quantum efficiency; detection of stimulated emission; and others. Advances and ideas will be discussed.

17:00 Quantum Technologies and Biology
Professor Martin Plenio, Ulm University

In this lecture I will discuss the beneficial relationship between quantum technologies and biology. I will point out how quantum dynamics may influence biological function, I will suggest new modes of interrogating biological systems by means of quantum technologies, especially diamond sensors and I will suggest ways to exploit self-organisation of biological systems for the creation of quantum information processors.

18:30 Drinks Reception – Balcony of dining hall, Robinson College

19:00 Workshop dinner & speech by **Professor Sir Peter Knight**

Thursday 19th March

SESSION I: Catalysis, Tunnelling and the Dynamics of Single Molecules

Session Chair: Professor Johnjoe McFadden, University of Surrey

09:00 H-tunnelling during enzyme-catalysed reactions

Dr Sam Hay, University of Manchester

Over the last 25 years, experimental studies describing enzymatic reactions with kinetic isotope effects that are significantly larger than the semi-classical limit have demonstrated that nuclear quantum mechanical tunnelling plays a role during catalysis. Here, the relative importance of tunnelling contributions to these reactions is considered and we find that the tunnelling contribution can confer a rate enhancement of up to approximately 1000-fold. Without tunnelling, a 1000-fold reduction in activity could seriously impair cellular metabolism, so we infer that tunnelling can be crucial to host organism viability.

09:45 Probes of quantum behaviour in organic molecules

Professor Vlatko Vedral, University of Oxford

A growing body of evidence suggests that biological processes could be utilising quantum coherence, superpositions, and even, in some cases, quantum entanglement to perform various tasks with higher efficiency [1]. I will first briefly summarize how I see the case for the existence of genuine quantum effects, including two of the most famous examples of biological processes: photosynthesis and magneto-reception [2]. I will then present the key features of modeling the flow of energy in complex systems [3]. The main challenge is to experimentally obtain a handful of parameters believed to be important for describing the interplay between coherence (within the system) and noise (arising due to the interaction of the system with its environment) [4]. I will present single molecule spectroscopy experiments we are currently undertaking in our laboratory to obtain a better understanding of quantum effects in biomolecules. Finally, I will explain how to set up experiments to test both quantum coherence [5] as well as thermodynamical properties of energy transport [6].

Acknowledgements. This work is supported by the Oxford Martin School, National Research Foundation (Singapore), the Ministry of Education (Singapore), the European Union, the Engineering and Physical Sciences Research Council (UK), the Fell Fund (Oxford) and the Leverhulme Trust (UK).

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10:30 **Coffee Break**

SESSION II: Theoretical modelling of biological nanostructures: from first principles to phenomena

Session Chair: Dr Ahsan Nazir, University of Manchester

11:00 **Linear-Scaling Electronic Structure Calculations applied to understanding Quantum Effects in Biological Systems**

Dr Nicholas Hine, University of Warwick

Elucidating vital biological processes often requires a detailed knowledge of the underlying electronic structure of the biomolecules involved, particularly those processes that harness electronic excitations, a category including photosynthesis, respiration and vision. Most spectroscopic probes also involve accessing excited electronic states, while proteins exhibiting fluorescence play a vital role as biomarkers across the biological and pharmaceutical sciences. However, the computational scaling of traditional electronic structure algorithms has limited quantum mechanical simulations of biomolecules to studies of small QM regions within a surrounding environment treated with empirical methods, an approach which is often inadequate to describe finely-tuned or long-ranged processes. In this talk, I will introduce ONETEP, a linear-scaling DFT package for large-scale electronic structure calculations [1], and discuss recent work applying it to biological molecules whose function harnesses quantum mechanics. I will discuss work on the Fenna-Matthews-Olson pigment-protein complex, which demonstrates the crucial role of quantum dynamics in photosynthetic exciton energy transfer. We have used linear-scaling DFT to calculate local pigment transition energies and interpigment coupling between optical transitions, enabling an ab-initio approach to simulating optical spectra [2]. I will also outline recent applications of the method to a diverse selection of biomolecules including hemoglobin [3], cellulose [4], and peptides involved in the formation of amyloid fibrils [5].

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11:45 Quantum delocalization directs antenna absorption to photosynthetic reaction centers

Professor Susana Huelga, Ulm University

Photosynthesis – the conversion of sunlight to chemical energy – is fundamental for supporting life on our planet. Despite its importance, the physical principles that underpin the primary steps of photosynthesis, from photon absorption to electronic charge separation, remain to be understood in full. Previously, electronic coherence within tightly-packed light-harvesting (LH) units or within individual reaction centers (RCs) has been recognized as an important ingredient for a complete understanding of the excitation energy transfer dynamics. However, the electronic coherence across RC and LH units has been consistently neglected as it does not play a significant role during these relatively slow transfer processes. Here, we turn our attention to the absorption process, which occurs on much shorter timescales. We demonstrate that the - often overlooked - spatially extended but short-lived excitonic delocalization across RC and LH units plays a relevant role in general photosynthetic systems, as it causes a redistribution of direct absorption towards the charge separation unit. Using the complete core complex of *Rhodospirillum rubrum*, we verify experimentally an 80 % increase in the direct optical absorption of the RC in situ as compared to isolated RCs. Numerical calculations reveal that similar enhancements can be expected for a wide variety of photosynthetic units in both plant and bacterial systems, suggesting that this mechanism is conserved across species and providing a clear new design principle for lightharvesting nanostructures.

12:30 Lunch

Session III: Quantum Sensing in the Natural World

Session Chair: Dr Erik Gauger, Heriot-Watt University

13:30 Electron spin changes during general anesthesia

Dr Luca Turin, Ulm University

One hundred sixty years after its discovery, the molecular mechanism of general anesthesia remains a notable mystery. A very wide range of agents ranging from the element xenon to steroids can act as general anesthetics on all animals from protozoa to man, suggesting that a basic cellular mechanism is involved. In this paper, we show that volatile general anesthetics cause large changes in electron spin in *Drosophila* fruit flies and that the spin responses are different in anesthesia-resistant mutants. We propose that anesthetics perturb electron currents in cells and describe electronic structure calculations on anesthetic-protein interactions that are consistent with this mechanism and account for hitherto unexplained features of general anesthetic pharmacology.

14:15 The effects of anthropogenic electromagnetic noise on the magnetic

compass of birds and its mechanistic consequences

Professor Henrik Mouritsen, University of Oldenburg

Migratory birds can use a magnetic compass to find their way, but how do they sense the reference direction provided by the geomagnetic field? In the past years, evidence has mounted that migratory birds use a light-dependent, radical pair-based mechanism to sense the axis of the geomagnetic field lines [1]. Recently, we could show that the magnetic compass of night-migratory birds is sensitive to anthropogenic electromagnetic fields being ca. 1000 times weaker than the current WHO guideline limits [2]. This result strongly indicates that the basic sensory mechanism underlying the magnetic compass of night-migratory songbirds should be based on quantum mechanical principles rather than classical physics. Neuroanatomical data have shown that magnetic compass information is detected in the eye and then processed in a small part of the thalamofugal visual pathway terminating in “Cluster N [3,4,5,6]. When Cluster N is deactivated, migratory European Robins can no longer use their magnetic compass, whereas their star compass and sun compass abilities are unaffected [6]. The lagena and associated pathways remained intact. Bilateral section of the trigeminal nerve had no effect on the birds’ ability to use their magnetic compass [6]. Thus, we are starting to get an understanding of magnetic compass sensing in birds, and several models and theoretical considerations suggests how the sense can work from a physical/quantum mechanical perspective. However, from my point of view, at the present time, the most important missing information needed to further advance our understanding of magnetoreception is the lack of biological and chemical experimental data, which are needed to evaluate and refine the presently suggested theories and models.

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15:00 **Panel Discussion and Q&A**

15:45 **Closing Remarks**

16:00 **CLOSE**

Biographies

Professor Jim Al-Khalili, University of Surrey

Professor Jim Al-Khalili is a theoretical physicist at the University of Surrey where he also holds a chair in the Public Engagement in Science. He received his PhD in nuclear reaction theory in 1989 from Surrey before working as Postdoctoral Fellow at UCL. He returned to Surrey and was awarded a five year EPSRC Advanced Research Fellowship in 1994. He was promoted to professor of physics in 2005. He has published widely on quantum scattering models to elucidate the structure of exotic (neutron halo) nuclei with his top two papers in the field having over 500 citations. Recently, he has applied his expertise to look at problems in quantum biology, such as proton tunnelling in point mutations in DNA. He has also published a number of papers on the history of science.

Jim is active as a science communicator and has written many popular science books, between them translated into 26 languages. He is a regular presenter of TV science documentaries as well as the weekly BBC Radio 4 programme, The Life Scientific. He is a recipient of the Royal Society Michael Faraday medal and the Institute of Physics Kelvin Medal and received an OBE in 2007 for 'services to science'. His latest book, with Johnjoe McFadden is Life on the Edge: The coming of age of quantum biology.

Dr Alex Chin, University of Cambridge

Dr Alex W Chin obtained his PhD in the Theory of Condensed Matter Group at the University of Cambridge and then undertook postdoctoral work at the Universities of Hertfordshire and Ulm. In 2012, he returned to Cambridge as one of the first Winton Advanced Research Fellows in the Physics Department's Winton Programme for the Physics of Sustainability. His current research interests include open quantum systems, photosynthesis, singlet fission, electron transport in supramolecular crystallites, electronic structure of photo-excited states and theories of various ultrafast spectroscopies.

Professor Gregory S. Engel, The University of Chicago, USA

Greg Engel was born in Pennsylvania in 1977. He obtained his A.B. from Princeton University in 1999 and his Ph.D. from Harvard University in 2004. Working under Prof. James Anderson at Harvard University, Greg designed and built ultrasensitive spectrometers to enable in situ measurements of atmospheric tracers and isotopic fractionation profiles of water vapor in the tropical tropopause transition layer. In 2005, he moved to UC Berkeley as a Miller Fellow to study photosynthetic energy transport. Working with Prof. Graham Fleming, Greg discovered coherent excitonic energy transfer in photosynthesis by observing quantum beating signals with 2D electronic spectroscopy. Greg is currently an Associate Professor at The University of Chicago in the Department of Chemistry, The James Franck Institute, and The Institute of Biophysical Dynamics. His research group focuses on new strategies to observe, measure, and control excited state reactivity. Using spectrometers of their own design, the Engel Group explores bio-inspired design principles for steering excitonic transport, open quantum dynamics, and photochemical reaction

dynamics. The group's scientific approach involves parallel efforts in theory, spectroscopy, biophysics, and synthesis. Greg is a current officer of the ACS Physical Chemistry Division and has served as chair of the ACS Biophysics subdivision. His research has been recognized with the Coblentz Award, National Security Science and Engineering Faculty Fellowship, Sloane Fellowship, Searle Scholar Award, Presidential Early Career Award in Science and Engineering, DARPA Young Faculty Award, AFOSR Young Investigator, DTRA Young Investigator, Dreyfus New Faculty Award, and Scientific American's SciAm 50 Award. Greg's teaching has been recognized with the Quantrell Award for Undergraduate Teaching and the Camille Dreyfus Teacher/Scholar Award.

Professor Sir Richard Friend, University of Cambridge

Richard Friend is the Cavendish Professor of Physics in the University of Cambridge. He has developed the semiconductor physics of pi-conjugated organic polymers, and his research group has demonstrated that these materials can be used in wide range of semiconductor devices. He has co-founded a number of Cambridge start-up companies to exploit these developments.

Professor Rienk van Grondelle, VU University, Amsterdam, The Netherlands

Rienk van Grondelle was born on December 6 1949 in Bussum, The Netherlands. After highschool (HBS-B in Hilversum, 1962-1967) he studied experimental physics at the VU University in Amsterdam between 1967 and 1973. His final research project was done under the guidance of Dr. Nico Westerhoff in the medical faculty of the VU and concerned the mechanics of bloodflow. He did his PhD between 1973 and 1978 in the Biophysics group of Leiden University under the supervision of Prof. Dr. Lou Duysens. His thesis "Primary and Cytochrome Reactions in Bacterial Photosynthesis" was awarded the degree cum laude. After a post doc at the University of Bristol (with Prof. Dr. Owen Jones) he returned to Leiden and became involved in ultrafast spectroscopy. In 1982 he moved back to the VU University, Department of Physics and Astronomy, where in 1987 he was appointed as full professor in Biophysics. Since then he has built a large group studying the early events in photosynthesis.

Rienk van Grondelle is one of the most influential experimental physicists working on the primary physical processes of photosynthesis world-wide. Using the tools of ultrafast spectroscopy he has made major contributions to elucidate the fundamental physical mechanisms that underlie photosynthetic light harvesting and charge separation. He has developed theoretical tools to infer the effective electronic and molecular structure and dynamics from complex spectroscopic data. His work recently led to a fundamental new understanding of light-driven charge separation in the oxygen evolving photosynthetic reaction center of plants. Using multi-dimensional electronic spectroscopy he was able to show that in photosynthesis ultrafast charge separation is driven by specific molecular vibrations that allow electronic coherences to stay alive. Five years ago he proposed an explicit molecular model for photoprotection and demonstrated that the major plant light harvesting complex operates as a nanoswitch, controlled by its biological environment. These results, of utmost importance for our understanding of photosynthesis, inspire technological solutions for artificial and/or redesigned

photosynthesis, as a possible route towards sustainable energy production on a global scale.

Dr Sam Hay, University of Manchester

Sam studied chemistry and biochemistry at the University of Otago (New Zealand) in 2000 before completing a PhD in biophysics at the Australian National University in 2004. He is interested in how biological processes – reactions and interactions – are governed by their underlying physics. The main focus of this work is the role of quantum mechanics during enzyme catalysis. This work employs both experimental and theoretical approaches, with an emphasis on instrument and method development and the development of new theory and models to underpin experiment.

Dr Nicholas Hine, University of Warwick

Nicholas Hine is an Assistant Professor in the Department of Physics at the University of Warwick, U.K. He was previously a Winton Advanced Research Fellow at the Cavendish Laboratory, Cambridge, and before that a Leverhulme Early Career Fellow at Imperial College London. During his PhD he worked with Prof Matthew Foulkes at Imperial on Quantum Monte Carlo methods. His research applies electronic structure methods to varied problems in materials physics, focussing on properties of nanostructures, including semiconductor nanocrystals, biological systems such as pigment-protein complexes, carbon nanomaterials, and the properties of defects in metal oxides. He is one of the main authors of the ONETEP Linear-Scaling DFT code, having made wide-ranging contributions to the code including developing new methodology for strongly correlated systems and electronic excitations, and dramatically increasing its parallel scaling.

Professor Susana Huelga, Ulm University, Germany

Studied theoretical physics in Salamanca (Spain) and got a doctorate from Oviedo University (Spain) under the supervision of prof. Emilio Santos. Moved to Claredon Laboratory, Oxford University, as a postdoc in 1996-97 and then to Imperial College London until 2000. I took up a position at the University of Hertfordshire in 2000 and became a Reader in Quantum Physics, moving to Ulm University in 2009 to take up a Professorship in Quantum Optics. My research interests focus on harnessing quantum effects in noisy environments and systems out of thermodynamical equilibrium.

Professor Niek van Hulst, The Institute of Photonic Sciences, Spain

Following study in Astronomy and Physics, I obtained my PhD (1986) in Molecular & Laser-Physics at the University of Nijmegen (the Netherlands), on microwave-laser double resonance molecular-beam spectroscopy. After research in non-linear optics of organic materials, integrated optics, atomic force and near-field optical microscopy, since 1997 full Professor in Applied Optics at MESA+ Institute for NanoTechnology, University of Twente (the Netherlands) with focus on single molecule detection, scanning probe technology and applications in molecular biology and chemistry.

In 2005, attracted by the Catalan open-minded quality-based science policy, I started as ICREA Research Professor and senior group leader at ICFO – the

Institute of Photonic Sciences – Castelldefels. I coordinated the Spanish CONSOLIDER program NanoLight.es. Recipient of an ERC Advanced Investigator Grant. City of Barcelona Prize 2010 for Scientific Investigation. Fellow of the Optical Society of America

My current interest is to control light interaction at the nanometer scale. To this end my group specializes on nano-antennas which confine light to far sub-wavelength hot spots, and on broad-band coherent control schemes to command light pulses at few fs timescale. By means of the optical antennas we address locally individual molecules, quantum dots and proteins, enhancing their excitation and managing emission rate, spectra, polarization and direction of single photon emission. By coherent control we explore the fs dynamics of individual molecules, nanoparticles and plasmonic hot spots. Recently we focus particularly on long-lived coherences in single light-harvesting antenna complexes at native conditions, to unravel the remarkably high efficiency of energy conversion in such natural molecular antennas.

Professor Sir Peter Knight, Imperial College London

Peter Knight is Senior Research Investigator in Physics at Imperial College and Senior Fellow in Residence at the Kavli Royal Society International Centre, Chicheley Hall and Past-President of the Institute of Physics. He retired in September 2010 as Deputy Rector (Research) at Imperial College where he was responsible for the College's research strategy. He was knighted in the Queen's Birthday Honours List in 2005 for his work in optical physics. Peter Knight was the 2004 President of the Optical Society of America and a member of their Board of Directors and a Director of the OSA Foundation. He was coordinator of the UK Nonlinear Optics Initiative and Editor of the Journal of Modern Optics and is Editor of Contemporary Physics. He is a Thomson-ISI "Highly Cited Author." He is a member of the UK Quantum Technology Initiative Strategy Advisory Board. He chairs the new Quantum Metrology Institute at the National Physical Laboratory and until the end of 2014 chaired the Advisory Board of the very successful EPSRC Innovative Manufacturing Centre at the University of Huddersfield. He is a member of the Advisory Board for the Winton Programme for the Physics of Sustainability in Cambridge.

Sir Peter was until December 2010 chair of the Defence Scientific Advisory Council at the UK Ministry of Defence, remains a Government science advisor and was a Council member of the Science and Technology Facilities Council until 2011. Sir Peter was also Chief Scientific Advisor at the UK National Physical Laboratory. His research centres on quantum optics, strong field physics and especially on quantum information science. He has won a number of prizes including the Thomas Young Medal and the Glazebrook Medal of the Institute of Physics, the Ives Medal of the OSA and the Royal Medal of the Royal Society. He has been a Visiting Professor at the University of Louvain-la-Neuve, a Humboldt Research Award holder at the University of Konstanz and a Visiting Scholar at the University of Texas at Austin and is a Research Professor at the University of Rochester. He is a Fellow of the Institute of Physics, the Optical Society of America and of the Royal Society. He is a Trustee of the Royal Institution and a member of Council at Sussex University.

Professor Johnjoe McFadden, University of Surrey

Molecular biologist and microbial geneticist working mainly on infectious diseases. BSc and PhD at University of London now working at University of Surrey, UK. Became interested in the role quantum mechanics in biology over a decade ago and, with Jim Al-Khalili, wrote a speculative paper on the potential involvement of proton tunnelling in mutation back in 2000. Published the book 'Quantum Evolution' in 2000, proposing a role for quantum mechanics in biology and co-authored, with Jim Al-Khalili, 'Life on the Edge: the Coming of Age of Quantum Biology', published in 2014. Currently investigating experimentally the role, if any, of proton tunnelling in mutation.

Professor Henrik Mouritsen, University of Oldenburg, Germany

All aspects of animal navigation from migration strategies of populations to the behavioural, physiological and molecular mechanisms enabling animals to navigate over thousands of kilometres. In recent years, we have primarily focused on understanding the physical, molecular, neuronal and behavioural mechanisms that enable birds to sense the Earth's magnetic field. This has also brought us into the field "quantum biology". Main model system: migratory birds.

Dr Alexandra Olaya-Castro, University College London

Alexandra did her undergraduate in Physics Education at Universidad Distrital Francisco Jose de Caldas (Bogota) and her MSc in Physics at Universidad de Los Andes in Bogota. During this time, she worked with Prof. Carlos Tejedor at Universidad Autónoma de Madrid, Spain and Prof. Pawel Hawrylak at the Institute for Microstructural Sciences in Ottawa, Canada. In 2002 she moved to the University of Oxford (Somerville College) to do her D Phil with Prof. Neil Johnson, funded by a Clarendon Fund Scholarship, an Overseas Research Student award, and a Somerville Senior Scholarship. She finished her doctoral studies in 2005 and subsequently obtained an independent Junior Research Fellowship at Trinity College, Oxford University. In November 2008 she was awarded an EPSRC Career Acceleration Fellowship to be held at University College London. She obtained a permanent Lecturer position in September 2011. Throughout her career Alexandra has made scientific contributions to the theoretical understanding of quantum coherence in a variety of quantum systems that include exciton condensates in quantum wells, multi-qubit systems embedded in optical cavities and photo-activated biomolecular systems.

Professor Martin Plenio, Ulm University, Germany

Martin Plenio is an Alexander von Humboldt Professor and Director of the Institute of Theoretical Physics at Ulm University as well as part-time Professor at Imperial College London. His research interests lie in the fields of quantum information science, quantum optics, quantum sensing and quantum effects in biology. In these fields he enjoys applying abstract theory to develop concrete experiments and applications.

He received his Diploma (1992) and PhD (1994) in Physics from Göttingen University and then moved to Imperial College London as a Fedor Lynen Humboldt Fellow in

1995, became Lecturer in 1998 and eventually a Full Professor of Quantum Physics in 2003. In 2009 he took up his present position following the award of the first Alexander von Humboldt Professorship by the German Ministry for Science and Technology. His research has been awarded with several prizes, including the Maxwell Medal and Prize 2004 of the British Institute of Physics, the Royal Society Wolfson Research Merit Award 2006, the Clifford Paterson Lecture for 2008 of the Royal Society, the Max Born Medal and Prize (2012), jointly awarded by the German Physical Society and the British Institute of Physics and in 2012 the first ERC Synergy grant. He is also the founding director of the Center for Quantum Biosciences with a state-of-the-art research facility that is currently being constructed with the help of federal and state funding exceeding €26 Million.

Dr Erwin Resiner, University of Cambridge

Erwin Reisner received his education and professional training at the University of Vienna (with Prof. Bernhard K. Keppler), the Massachusetts Institute of Technology (with Prof. Stephen J. Lippard) and the University of Oxford (with Prof. Fraser A. Armstrong) before starting his independent career as a University Lecturer at Cambridge and Fellow of St. John's College in 2010. He holds an EPSRC Career Acceleration Fellowship, heads the Christian Doppler Laboratory for Sustainable SynGas Chemistry and is a co-director of the EPSRC Centre for Doctoral Training in Functional and Sustainable Nano. His group develops artificial photosynthesis by combining chemical biology, synthetic chemistry and materials chemistry.

Dr Luca Turin, Ulm University, Germany

Luca Turin is currently Visiting Professor in the Institute of Theoretical Physics in Ulm. He got a PhD in Physiology and Biophysics from UCLondon in 1978 and has worked at the CNRS in France, UCL, in the private sector as CTO of a US molecule discovery company, at MIT and at the Alexander Fleming Institute in Athens, Greece.

Professor Vlatko Vedral, University of Oxford

Vlatko Vedral is a professor of quantum information theory at the University of Oxford and professor of physics at the National University of Singapore (where he is a PI at the Centre for Quantum Technologies). He is the Director of the Oxford Martin School institute on "bio-inspired quantum technologies". This explores the exciting possibility that living systems are subject to useful quantum effects, with a view to deriving and reverse-engineering architectures to inspire future quantum technologies that will help address serious challenges facing humanity in the 21st century. He has received numerous awards in recognition for his contribution to the development of the field, including the Royal Society Wolfson Research Merit Award and the World Scientific Medal and Prize. He has over 220 publications on quantum physics and collaborates in many inter-disciplinary international networks.

Posters and Abstracts

Alexander Fokas, University of Cambridge

“The role of Allosteric Communication in Reducing Uncertainty during Energy Transfer”

Proteins participate in virtually all cellular processes and are employed in photosynthetic organisms to harvest sunlight. The FMO complex is a trimer of monomers that each sequester seven optically active molecules (pigments). The activity of these pigments, which is dominated by the protein environment, are central to the process of excitation energy transfer. The interest generated by this molecular machine is related to the observed, and remarkable, quantum yield. A shift in focus from the pigment properties to the protein environment followed the observation that coherent energy transfer was supported in this biological system. Indeed, proteins are not static molecules. They are known to form mobile kinetic species that can be better approximated using conformational ensembles. The following study has employed FIRST to study the flexibility in the protein network. A module (FRODA) within FIRST was then employed to generate the accessible conformational states. The analysis revealed correlated motions between functionally relevant structures in the protein. Importantly, correlations were also identified between pigments that previously were found (experimentally) to be excitonically coupled. The excitonic coupling between the pigments was approximated using a charge density coupling analysis. The inclusion of motion revealed coupling between pigment three and seven, which did not emerge in previous work involving the static structure. We believe that low variation in conformational states (due to the rigid structure) and the excitonic coupling (due to correlated motions) provides evidence that the protein motion has evolved to support subtle quantum behaviours in the disordered protein environment.

Jake Iles-Smith, Imperial College London

“Energy transport dynamics in an incoherently molecular dimer”

Many experiments have now confirmed the presence of quantum coherence in photosynthetic energy transport systems, however the precise origin of this coherence remains an open question. For example, there exists several arguments in the literature that this coherence is not an inherent property of photosynthetic complexes, but is instead generated by the coherent light-sources used in experiments.

In this work we consider the effect incoherent driving and coupling to a vibrational environment has on the energy transfer dynamics in a molecular dimer system. To do this, we make use of the reaction coordinate formalism to describe the vibrational environment when the environments' correlation time is long. Here, important environmental degrees of freedom are incorporated into a new effective system, which may be modelled straightforwardly using standard perturbative techniques. From this we demonstrate that strong coupling between a system and its vibrational environment leads to the emergence of both dynamical and steady state coherence in the energy eigenbasis.

E.A. Hemmig, **Philip Mair**, C. Creatore, F.A.Y.N. Schröder, M.A. Parker, A. Rao, A.W. Chin, and U.F. Keyser, **University of Cambridge**
“Exploring quantum effects in biologically inspired DNA origami Nanostructures”

The DNA origami technique has emerged as a powerful ‘bottom-up’ approach for the assembly of two- and three-dimensional nanostructures with tailored geometries and chemical addressability [1]. Our research efforts are focused on the functionalisation of DNA origami structures by attaching fluorescent dye molecules with base-pair accuracy. Our aim is to explore the possibilities of DNA origami as a versatile platform to design sophisticated, multicomponent nanoarchitectures for the study of quantum effects underlying light-harvesting in photosynthesis [2]. Here, we introduce a biologically inspired DNA origami design consisting of a ring of donor fluorescent dyes surrounding an acceptor core on a flat, square-shaped DNA origami platform (Figure 1). Steady-state fluorescence analyses of various donor-acceptor geometries revealed that the light-harvesting ability is highly enhanced by increasing the number of adjacent donors.

Furthermore, we demonstrate the possibility of fine-tuning the observed antenna effect by varying the concentration of Mg^{2+} ions in the buffer solution. In conclusion, these initial results clearly show the potential of the DNA origami technique to build artificial mimics of light-harvesting complexes with exquisite control over donor-acceptor geometry.

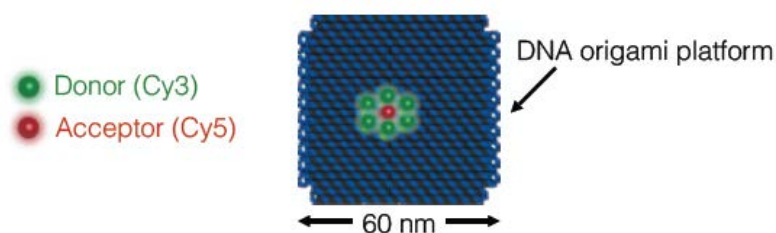


Figure 1: Biologically inspired arrangement of donor and acceptor fluorescent dyes in a ring-like structure on a flat, square-shaped DNA origami platform.

[1] P. Rothemund. Folding DNA to create nanoscale shapes and patterns. *Nature* 2006, 440, 297-302.

[2] C. Creatore, M. A. Parker, S. Emmott, A. W. Chin. Efficient biologically inspired photocell enhanced by delocalized quantum states. *Physical Review Letters* 2013, 111(25), 253601.

Sarah Morgan, University of Cambridge

“Real-time Observation of Multiexcitonic States Mediating Ultrafast Singlet Fission Using Coherent 2D Electronic Spectroscopy”

2D optical spectroscopy allows unprecedented insight into the ultrafast electronic and vibrational dynamics of a range of molecular and condensed-matter systems, including biological light-harvesting systems and organic thin films. However, separating out this information is often non-trivial, particularly establishing the difference between signals of vibrational, electronic and mixed vibrational and electronic origins.

Here we analyse recent 2D spectroscopy data for pentacene, where the ultrafast (<100fs) decay of a singlet exciton into a spin-correlated (maximally entangled) pair of (dark) triplet excitons can be observed. This process, known as singlet fission, is an area of active research, as the triplet pair subsequently decays to independent, long-lasting triplet excitations which can each generate a charge(1,2). Therefore a fission-based photodiode has a theoretical quantum efficiency of 200%. We show that the key intermediate state can be resolved in 2D spectroscopy due to both vibrational coupling and excited state absorption, providing new insight into how fission proceeds. This work is a concrete example of how 2D spectroscopy can help to establish the underlying physical mechanisms in a real physical system and many of the techniques used here could also be applied to other organic molecular systems, notably biological light-harvesting systems.

[1] Chan, Ligges, Jailaubekov, Kaake, Miaja-Avila and Zhu, *Science*, 334, pp. 1541–1545, 2011

[2] Wilson, Rao, Clark, Kumar, Brida, Cerullo and Friend, *JACS*, 133, pp. 11830–11833, 2011

Aleksandar Sebesta, Alexander Weigel, Philipp Kukura, **University of Oxford**
“Single Molecule Dynamics Under Shaped Femtosecond Illumination in the One-Photon Limit”

Femtosecond spectroscopy is key to understanding or even controlling ultrafast molecular motion and relaxation after optical excitation, but experiments have up to now been largely restricted to ensemble measurements. Ultimately the goal is to reach single molecule sensitivity to study individual particles in their micro or nano-environment. Recent results [1,2] have been interpreted in terms of electronic coherence and wavepacket interference, and it was suggested that quantum control is possible on the single-molecule level. There has been a long-standing debate if the specific shape of a pulse can modify the absorption properties of a chromophore, even if only a single photon is absorbed. Here we present different coherent control experiments in the weak field regime on single molecules.

Starting with 11 fs pulses from a home-built 8 MHz white light laser we used a spatial light modulator to conduct pulse pair, pulse train, and closed loop coherent control experiments. In a first experiment, a terylene molecule was excited with two identical transform limited pulse copies, with varying inter-pulse delays (Figure 1a). Monitoring the delay dependent fluorescence intensity yields traces shown in Figure 1b. Taking the difference and the sum of the phase-cycled traces in (Figure 1b), we separate the phase-dependent oscillations (difference) from the phase-independent (sum) background. Fourier transformation of difference trace (Figure 1c) yields the fluorescence excitation spectra of the single molecule, closely resembling the ensemble absorption spectrum in toluene. The oscillatory modulations can solely be explained by the delay-dependent interference of the excitation pulses without the need for more complicated explanations like electronic coherence phenomena and wavepacket interference proposed in recent publications.[1,2] Fourier transformation of the oscillatory part directly yields the single molecule fluorescence

excitation spectrum in Figure 1d.

Ultimately we present the first close loop coherent control experiment on a single molecule (Figure 2), which probes if any non-trivial phase in the excitation is capable of changing the excitation probability. A genetic algorithm searches for optimal control phases with the fluorescence intensity as control parameter. The fitness is defined as the relative change of the fluorescence intensity of a compressed pulse compared to a pulse with an optimized phase. The resulting traces (Figure 2) show no change from the initial level of fluorescence intensity in both the maximization and minimization experiments.

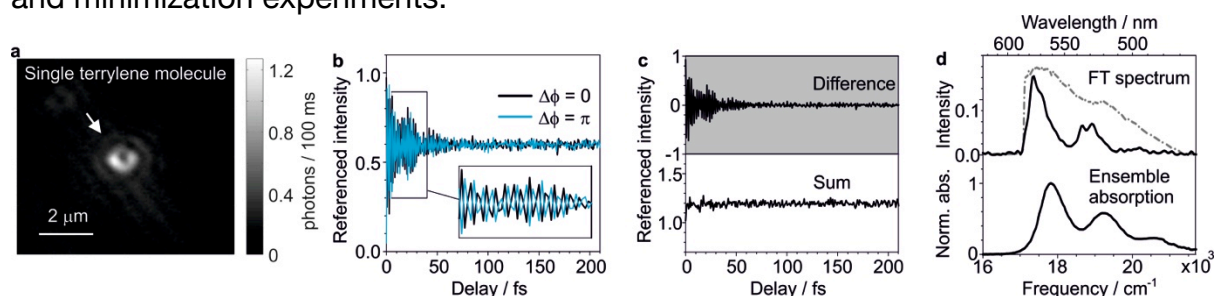


Figure 1. **a** Widefield fluorescence image of a single terrylene molecule. **b** Delay dependent fluorescence intensity trace for a pulse pair experiment. **c** Difference and sum of the fluorescence traces in **b**. **d** Fluorescence excitation spectra of the single terrylene molecule obtained by Fourier transformation of the difference trace, and comparison to the ensemble absorption.

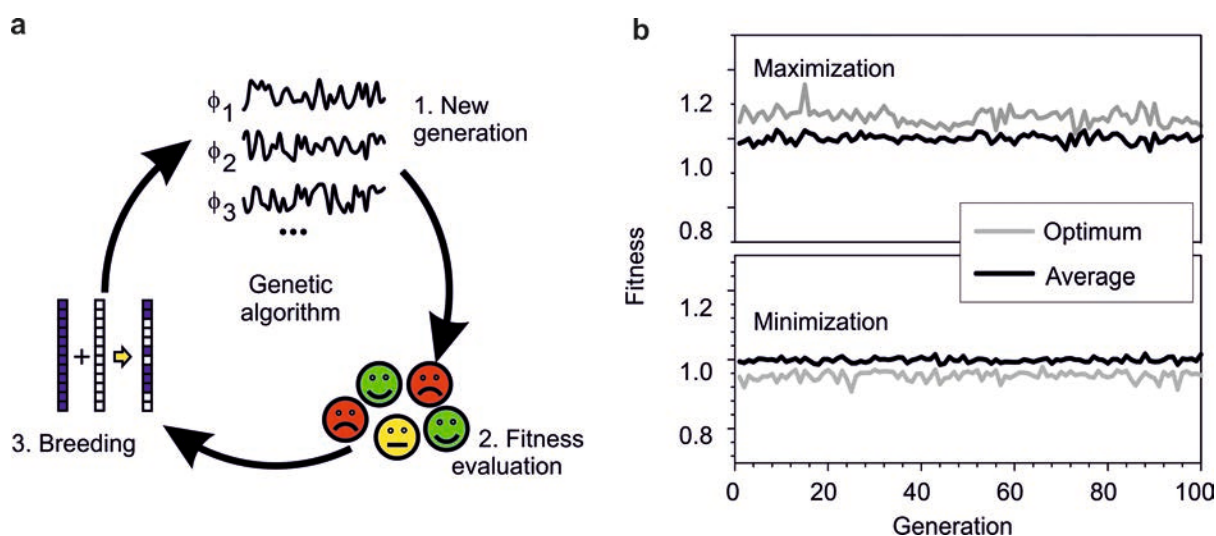


Figure 2 **a** Schematic of a closed loop coherent control experiment. In a first step random phase masks are generated, subsequently the fitness of each mask is tested against criteria (minimization or maximization of fluorescence intensity). The best phase masks are chosen from the pool and bred with new random phase masks. **b** The outcome of the maximization and minimization experiment on a single terrylene molecule as in Figure 1a.

[1] D. Brinks *et al.*, “Ultrafast dynamics of single molecules”, Chem. Soc. Rev. (2014).

[2] D. Brinks *et al.*, “Visualizing and controlling vibrational wave packets of single molecules”, Nature 465, 905-909 (2010).

Florian Schroeder, University of Cambridge

“Many-body quantum dynamics simulated with Matrix Product States”

We present a variational matrix product states (VMPS) implementation which combines several state of the art techniques to accurately compute ground state properties and dynamics of many-body Hamiltonians, in particular the spin-boson model (SBM).

Environmental spectral densities can be either discretized with well established logarithmic discretization schemes and mapped onto a Wilson chain, or directly mapped onto the chain without discretization using orthogonal polynomials. This method turns out to be exact and equivalent to a discretization with infinitely fine resolution.

Time evolution is implemented in a Dirac-Frenkel style time-dependent variational principle (TDVP) instead of the commonly used Suzuki-Trotter decomposition of the time evolution operator. This allows optimal time evolution even for long-range 1D-Hamiltonians. Computations in the weak and strong coupling regime of the ohmic and sub-ohmic SBM are compared to contemporary numerical results to prove the capabilities of the implementation.

Sam Smith, University of Cambridge

"Ultrafast charge separation in organic solar cells, simple models and detailed treatments."

Traditionally, charge transport in organic semiconductors and molecules has been described by incoherent hopping models like the celebrated Marcus theory. However a number of recent experiments have shown that electrons and holes at interfaces between donor and acceptor phases separate on extremely short, sub 100fs timescales; something hopping models cannot explain. In this work we formulate a simple account of ultrafast charge separation, arising from a short-lived partially coherent dynamical regime. We go on to demonstrate the compatibility of our model with the detailed electronic bandstructure of PCBM, the most popular electron acceptor in organic photovoltaics.

Richard Stones, University College London

“Current Statistics Reveals Reduced Noise in Vibration-Assisted Charge Separation in Photosynthetic Reaction Centres”

Photo-induced charge separation in the photosystem II reaction centre (PSIIRC) of higher plants occurs with almost unit quantum efficiency and is thought to be aided by coupling to intra-molecular vibrational modes. Properties like these make photosynthetic systems interesting as potential components in bio-hybrid nano-electronic devices. We propose a theoretical photocell device based on PSIIRC and study the full counting statistics of the current passing through it. We observe three interesting features in the behaviour: a reduction in current on inclusion of high energy modes in the spectral density, optimality of temperature and dynamical channel blockade in certain parameter regimes.

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Professor	Vlatko	Vedral	University of Oxford
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Notes

