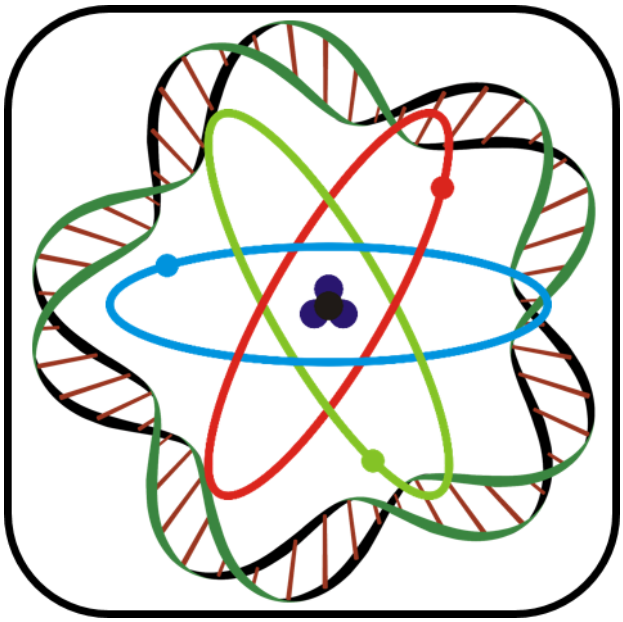
Quantum Biology Workshop
Programme

21 – 22 July 2017
University of Surrey, UK
Lecture Theatre M



This meeting is part of a series of Focussed Workshops delivered through the EPSRC NetworkPlus in 'Understanding the Physics of Life 2'.

INTRODUCTION

Quantum biology is an interdisciplinary field investigating non-trivial quantum effects, such as long lived quantum coherence, that play a role, at the molecular level, within living cells. The field has emerged in recent years as a result of a number of surprising experimental discoveries, such as quantum coherence in photosynthesis, quantum tunnelling in enzyme action and olfaction, possible quantum entanglement in avian navigation and several other areas.

There are a number of universities in the UK that currently have activities in QB; among them are Surrey, UCL, Oxford, Cambridge, Bristol, Southampton, Liverpool, Manchester and Glasgow. However, in most these institutions, the activity is that of one or two researchers rather than a large, well-funded, research group. There have been three recent UK meetings on QB. The first, in 2011, was held at the Kavli Centre of the Royal Society, which focussed mainly on quantum coherence effects in photosynthesis (royalsociety.org/events/2011/quantum-coherent-energy/). The second was a workshop held at Surrey in 2012 (www.ias.surrey.ac.uk/workshops/quantumbiology). There was also a smaller meeting in Cambridge in 2015 (www.winton.phy.cam.ac.uk/QT_bio_workshop). In the light of significant recent interest in QB, we feel it is timely to run a new workshop under the umbrella of the EPSRC funded Physics of Life Network (PoLNet2).

Over the past few years, quantum biology has grown from a speculative, some would even say controversial, field to one where exciting opportunities are being found, particularly as it bridges the vacuum between two other recently well-funded areas: quantum technologies and synthetic biology. The aim of this workshop is more than to simply allow the small but growing QB community in the UK to update each other on their work, but rather to bring the disparate communities together, to help create a coherent network of activities and researchers in the UK and to catalyse sizeable research programmes in a sustainable way as well as to sharpen research questions, methodologies, and disciplines. To this end, a range of stakeholders and interested parties have also been invited to participate and to introduce them to the research opportunities and potential applications offered by QB. We believe strongly that there is capability for the UK to become a world leader in the field. The main theme of current work in QB is to look for and understand 'unambiguous signatures of quantum effects in biological systems'.

Workshop chairs:

Jim Al-Khalili

Johnjoe McFadden

DAY 1: Friday 21 July 2017

Venue: Lecture Theatre M

0900 Registration and coffee

0925 Welcome from Jim Al-Khalili

Session 1 (Chair: Johnjoe McFadden)

0930 **Peter Weightman** (Liverpool) – Experimental tests of the Frohlich hypothesis

1015 **Judy Armitage** (Oxford) – A biased random walk: controlling the rotation of a 45nm ion driven nanomachines

1100 Coffee break

1130 **Peter Hore** (Oxford) – Avian magnetoreception: a quantum compass needle

1215 **Alex Jones** (Manchester) – Structure, function and signalling in cryptochrome-dependent animal magnetoreception

1300 Lunch

Session 2 (Chair: Jim Al-Khalili)

1400 **Sam Hay** (Manchester) – Proton tunnelling in enzymes

1440 **Daniel Kattnig** (Exeter) **–** The quantum magnetic compass: unexpected consequences of chemical reactivity

1505 **Johnjoe McFadden** (Surrey) – Stochasticity and cell division: is quantum noise involved?

1530 Coffee break

1600 **Rudo Roemer** (Warwick) – Electronic transport in DNA and the interplay of mutations and electronic properties in disease-related genes

1640 **Animesh Datta** (Warwick) – Energy transport in photosynthetic systems

1700 End of Day 1

1900 Dinner at Olivo Restaurant (53 Quarry St, Guildford GU1 3UA), arrival by 18:30

DAY 2: Saturday 22 July 2017

Venue: Lecture Theatre M

0830 Coffee

Session 3 (Chair: Stephen Till)

0900 **Alexandra Olaya-Castro** (UCL) – Photon and electron counting statistics: a tool box for probing quantum effects in biomolecules

0945 **Jose Jimenez** (Surrey) – Experimental sequence space exploration of a fitness landscape of short RNA molecules

1030 Coffee break

1100 **Jakub Sowa** (Oxford) – Environment-Assisted Transport through Single-Molecule Junctions

1130 **Daniel Cole** (Newcastle) – Towards ab initio Modelling of Quantum Effects in Biology

1200 **Nick Werren** (Surrey) – Memory effects in Open Quantum Systems

1230 Lunch

Session 4 (Chair: Lee Poeppelman)

1330 **Peter Wright** (Imperial College) – Non-optical nanoscale functional imaging for studying ion channels and receptors

1415 **Open discussion I:** Research questions and challenges

1500 Coffee break

1530 **Open discussion II:** Networking, funding opportunities and the way ahead

1600 End of workshop

SPEAKERS: DAY 1

SESSION 1

Experimental tests of the Frohlich hypothesis

Peter Weightman, Physics Department, University of Liverpool

Many decades ago Herbert Frohlich hypothesised that long wavelength modes of electromagnetic radiation play an important role in biological self-organization and mediate the formation of a coherent state [1]. Frohlich argued that the self-organization of living systems is maintained by a flow of free energy through a coherent exited state maintained by metabolic processes. He predicted that under appropriate conditions biological sys tems can support coherent excitations in the range 109 to 1012 Hz, a region now referred to as terahertz radiation (1 THz ~ 300 microns ~ 0.004 eV). This hypothesis is very relevant to the question as to whether or not quantum mechanics plays a non-trivial role in living systems an idea that has been discussed by physicists for decades and often dismissed by biologists due to a lack of conclusive experimental evidence. It is been difficult to devise tests of Frohlich's hypothesis because until relatively recently there have been no strong sources of THz radiation. Fortunately strong sources of THz radiation are now becoming available through the development of accelerator driven light sources [2]. The lecture will describe the results of experiments designed to test the Frohlich hypothesis [3,4] and set out opportunities for future experiments.

References
1 Frohlich Int. J. Quantum Chem. 2 641 (1968)
2 Weightman, Physical Biology. 9 053001 (2012)
3 Williams et. al. Phys. Med. Biol. 58 373 (2013)
4 Demidova et. al. Bioelectromagnetics 34 15 (2013)

References
1 Alexandrov et. al. Phys. Lett. A 374 1214 (2010)
2 Weightman, Physical Biology 9 053001 (2012)
3 Williams et. al. Phys. Med. Biol. 58 373 (2013)
4 Titova et. al. Nature Scientific Reports 3 : 2363 (2013)
5 Demidova et. al. Bioelectromagnetics 34 15 (2013)

Bio:

Peter Weightman (PW) is a Professor of Physics in the University of Liverpool and a former Director of the Interdisciplinary Research Centre in Surface Science. He was awarded the British Vacuum Council Senior Prize (2011), the Mott Medal of the Institute of Physics (2006), the Riviere Prize of the UK Surface Analysis Forum (2000) and the Science Prize of the UK ESCA Group (1990). With two colleagues he secured the initial funding for the ALICE accelerator at Daresbury and served on its project board. He subsequently received funding to construct a unique high peak power terahertz beamline and tissue culture facility on ALICE, which he used to study mechanisms of biological organization and investigate the Frölich hypothesis. Peter is currently leading a team that established a scanning near field microscope on the infrared free electron laser on ALICE and this is being applied to the study of esophageal, prostate and cervical cancers. The research featured on the BBC today programme and can be found on Youtube at www.youtube.com/watch?v=d7Lbyuqor8A

A biased random walk: controlling the rotation of a 45nm ion driven nanomachines

Judy Armitage, University of Oxford

Bacteria swim in environments which are all viscosity and no inertia, and are too small to sense a spatial gradient. They swim by rotating rigid helical flagella. Rotation is driven by a transmembrane rotary motor with the energy supplied by the transmembrane proton or sodium gradient. If driven by protons the 45nm rotor spins at ~300 Hz and is sodium at over ~100Hz. Rotation is caused by the ions moving through wall anchored stator proteins causing a structural change in those proteins. This changes the relationship between a charged interface of the stator and the rotor and movement is caused by a combination of electrostatic interaction and a steric push. There are ~26 steps per revolution and each uses about 52 protons, but whether it is tight or loose coupled is unclear. The motor is not however a stable nanomachine, but the stator proteins are exchanging with diffusing pools and the number of engaged stators reflects the external viscosity, and therefore required torque. The rotor can switch between CCW and CW rotation, with the switch driven by small signalling proteins binding to the base of the rotor, probably driving conformational spread in the rotor ring. Bacteria respond to a small percentage change in effector concentration over background concentrations of 5-6 orders of magnitude, and can integrate 10s of external and internal signals. The sensory system has a memory, comparing now with 2 sec ago and controlling the frequency of motor switching in response. The sensitivity and gain results from a network of thousands of interlinked, adaptive receptors operating as "signalling teams". The signals serve to bias the overall swimming in a favourable direction, and the variation in size and state of the receptor complexes causes a stochastic response in the population, effecting survival and growth.

Bio:
Judy Armitage a bacterial physiologist who has investigated aspects of bacterial responses to their environment for around 40 years. She is particularly interested in how bacteria swim and how that swimming is controlled to bias movement towards an optimum environment for growth. Her group use a very wide range of approaches and collaborate with experimental physicists and with mathematical modellers. She is a Member of EMBO, Fellow of the European and the American Academies of Microbiology and a Fellow of the Royal Society.

Avian magnetoreception: a quantum compass needle

Peter Hore, University of Oxford

Most physical scientists would probably be sceptical about the suggestion that a chemical reaction could respond to a magnetic field as weak as that of the Earth. After all, the interaction of a molecule with a ca. 50 mT magnetic field is more than a million times smaller than the thermal energy (kBT) at physiological temperature. Nevertheless, the kinetics of certain chemical reactions are magnetically sensitive. The key molecular species are pairs of transient free radicals whose electron-nuclear spin systems evolve coherently under the influence of internal and external magnetic interactions.

I will discuss the proposal that the coherent quantum spin-dynamics of photo-induced radical pairs in cryptochromes (photo-active proteins) could be the mechanism of the light-dependent magnetic compass sense of migratory birds.*

*The radical-pair mechanism of magnetoreception
P. J. Hore and H. Mouritsen
Annu. Rev. Biophys., 45 (2016) 299-344.

Bio:

Professor of Chemistry, Department of Chemistry, University of Oxford, UK.
Fellow and Tutor in Chemistry, Corpus Christi College, University of Oxford, UK.
Research interests: spin chemistry, avian magnetoreception, radical pair mechanism, magnetic field effects on chemical reactivity, spin dynamics.

Structure, function and signalling in cryptochrome-dependent animal magnetoreception

Alex R. Jones, School of Chemistry and Manchester Institute of Biotechnology, The University of Manchester and National Physical Laboratory

Photomagnetoreception in the fruit fly, Drosophila melanogaster, is dependent on the blue-light photoreceptor protein, cryptochrome (CRY), which has also been implicated in avian magnetoreception.

For there to be a behavioural response to a magnetic field, the effect on the primary magnetoreceptor needs to ultimately impact the nervous system. I will present data that show a significant impact on a measure of central nervous system response in Drosophila larvae of a combination of magnetic fields and specific wavelengths of light. This effect is CRY-dependent. Exposure of CRY-expressing neurons in the Drosophila brain to blue light is known to result in a depolarisation of the membrane and increased action potential firing. Electrophysiology data from single motoneurons show these effects of CRY and light can be potentiated by exposure to magnetic fields.

The chemical compass model of CRY-dependent magnetoreception is currently discussed in terms of a quantum effect of magnetic fields on radical pair chemistry within the protein. These radical pairs are thought to be generated by electron transfer chemistry triggered by photoexcitation of the blue-light chromophore, flavin adenine dinucleotide (FAD), which is bound to CRY. I will present data that describe the structural features of CRY that are necessary for the secure binding of FAD. These data will be discussed in the context of differential binding of FAD by CRY from different animals. The implications this has for the role of CRY in animal magnetoreception will be considered.

Bio

Alex is currently head of the Mechanistic and Applied Photobiology research group in the School of Chemistry at The University of Manchester. His research interests are broadly concerned with the interaction between electromagnetic radiation – be that light or magnetic fields (or both) – and (bio)molecules. Using mainly laser-based techniques his group studies the biophysical mechanism of photo- and magneto-receptor proteins that depend on a range of chromophores. They then either track the initial physical processes to a biological outcome or translates the fundamental mechanistic knowledge into bio-inspired technologies. In August 2017, Alex will move to a new position at the National Physical Laboratory.

SESSION 2

Proton tunnelling in enzymes

Sam Hay, University of Manchester

Enzyme-catalysed H-transfer reactions (where H is a proton, hydrogen atom, or hydride) are ubiquitous, yet fundamental details of these reactions remain unresolved. Quantum mechanical tunnelling of the transferred H appears to play a role under ambient/physiological conditions, which have been assumed to be too warm, wet and noisy for most non-trivial quantum mechanics to play a significant role. In the case of enzyme catalysed reactions, H transfer likely occurs by a 'corner cutting' mechanism where tunnelling occurs from a thermally-activated 'tunnelling ready configuration' [1]. Much work is now focused on the role of protein vibrations during these reactions, using a range of experiments including (ultrafast) spectroscopy and stable isotope effect measurements. A case can be made for the combination of multiple experimental and computational/theoretical approaches when studying these reactions and several examples will be given [2,3], including recent work aimed to answer whether evolution has selected for enhanced quantum mechanical tunnelling during enzyme catalysis.

[1] S Hay, NS Scrutton (2012) Good vibrations in enzyme-catalysed reactions, Nature chemistry 4, 161-168

[2] JE Longbotham, SJO Hardman, S Görlich, NS Scrutton, S Hay (2016)
Untangling heavy protein and cofactor isotope effects on enzyme-catalyzed hydride transfer, J Am Chem Soc 138, 13693-13699

[3] M Delgado, S Görlich, JE Longbotham, NS Scrutton, S Hay , V Moliner, I Tuñón (2017)
Convergence of Theory and Experiment on the Role of Preorganization, Quantum Tunneling, and Enzyme Motions into Flavoenzyme-Catalyzed Hydride Transfer, ACS Catal 7, 3190–3198

Bio

Sam first studied biochemistry and chemistry at the University of Otago, New Zealand (2000), before completing his PhD in biophysics at the Australian National University (2004). He then spent a year at Stockholm University as a Wenner-Gren visiting postdoctoral fellow (2004-2005) before moving to the University of Manchester to work as a postdoctoral research associate studying enzyme-catalysed H-transfer. In 2010 he set up his own group at the University of Manchester after receiving a BBSRC David Phillips fellowship. A main focus of his 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

The quantum magnetic compass: Unexpected Consequences of Chemical Reactivity

Daniel R. Kattnig[1] and P. J. Hore[2]
[1]*University of Exeter, Living Systems Institute*
[2]*Physical and Theoretical Chemistry Laboratory, University of Oxford*

Birds have a remarkable ability to obtain navigational information from the Earth's magnetic field during their long migratory voyages. The primary detection mechanism of this compass sense is uncertain but appears to involve the quantum spin dynamics of radical pairs formed transiently by photo-induced electron transfer reactions in the flavor-protein cryptochrome. It is puzzling that in many respects the compass performance in animals surpasses the predictions of model calculations [1], suggesting the presence of a powerful, yet unknown, amplification process. This prompted us to seek quantum and classical amplification mechanisms.[2,3] Here, we report on a surprising effect associated with spin-selective reactivity that can vastly enhance the performance of the quantum magnetic compass.

Based on model calculations, we propose a new mechanism of magnetoreception in cryptochromes that features a spin-selective electron transfer reactions of one of the radicals of the primary pair with spin-bearing scavenger (chemical Zeno effect).[4,5] The new scheme offers clear and important benefits such as a greatly enhance sensitivity to a 50 μT magnetic fields (by up to two orders of magnitude in the relative anisotropy) and magneto-sensitivity for radicals that are more than 2 nm apart. This means that radical pairs that are too far apart to undergo spin-selective recombination reactions could also be viable magnetic compass sensors and that the detrimental effects of inter-radical exchange and dipolar interactions can be minimized. Even more surprisingly, the effect immunizes the sensor to fast decoherence processes in one of the radicals. As a concequence, magnetic field effects of radical pairs involving swiftly spin-relaxing species, such as superoxide, are no longer be precluded.

[1] D. R. Kattnig, I. A. Solov'yov and P. J. Hore, Phys. Chem. Chem. Phys., 18 (2016) 12443-12456; [2] D. R. Kattnig, E. W. Evans, V. Dejean, C. A. Dodson, M. I. Wallace, S. R. Mackenzie, C. R. Timmel and P. J. Hore, Nature Chem. 8 (2016) 384-391; [3] D. R. Kattnig, J. K. Sowa, I. A. Solov'yov and P. J. Hore, New J. Phys., 18 (2016) 063007; [4] A. S. Letuta & V. L. Berdinskii, Doklady Physical Chemistry 463, 179-181 (2015). [5] D. R. Kattnig & P. J. Hore, Sci. Rep. submitted; http://arxiv.org/abs/1706.04564.

Stochasticity and cell division: is quantum noise involved?

Johnjoe McFadden, University of Surrey

Genetically-identical living cells nevertheless exhibit a wide variation in phenotypic properties, a phenomenon known phenotypic variation, which is involved in a wide range of phenomena including resistance of bacteria to antibiotics, metabolic bistability1, resistance of tumours to anti-cancer drugs2, development of immunity3, cell differentiation, development and aging4. However, its mechanistic origin remains obscure. Stochastic gene expression is certainly involved5, but stochastic protein expression, stochastic differences in epigenetic modification and weak ergodicity breaking6 may also be involved. These are all classical mechanisms; however, many biological processes are driven by very small numbers of molecules so it is possible that quantum fluctuations may also play a role. In this talk I will explore the role of stochasticity in biology, with particularly reference to cell division, and discuss how quantum fluctuations may be recognized.

Reference:

1 Mannan, A. A. et al. Integrating Kinetic Model of E. coli with Genome Scale Metabolic Fluxes Overcomes Its Open System Problem and Reveals Bistability in Central Metabolism. PLoS One 10, e0139507, doi:10.1371/journal.pone.0139507 (2015).

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4 Raj, A. & van Oudenaarden, A. Nature, nurture, or chance: stochastic gene expression and its consequences. Cell 135, 216-226 (2008).

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6 Rocco, A., Kierzek, A. M. & McFadden, J. Slow protein fluctuations explain the emergence of growth phenotypes and persistence in clonal bacterial populations. PLoS. ONE 8, e54272, doi:10.1371/journal.pone.0054272 [doi];PONE-D-12-27885 [pii] (2013).

Bio

Johnjoe McFadden is a systems biologist, bionanotechnologist and microbial geneticist with interests in infectious disease, particularly tuberculosis and meningitis. He also has a strong interest in quantum biology writing the first popular science book arguing for a central role of quantum mechanics in biology, Quantum Evolution, in 2000, and then Life on the Edge, with Jim Al-Khalili, in 2014.

Electronic transport in DNA and the interplay of mutations and electronic properties in disease-related genes

Rudolf A. Roemer, University of Warwick

Electronic properties of DNA are believed to play a crucial role in many phenomena in living organisms, for example the location of DNA lesions by base excision repair (BER) glycosylases and the regulation of tumor-suppressor genes such as p53 by detection of oxidative damage. However, the reproducible measurement and modelling of charge migration through DNA molecules at the nanometer scale remains a challenging and controversial subject even after nearly two decades of intense efforts. Here we show, by analysing 162 disease-related genes from a variety of medical databases with a total of almost 20, 000 observed pathogenic mutations, a significant difference in the electronic properties of the population of observed mutations compared to the set of all possible mutations. Our results have implications for the role of the electronic properties of DNA in cellular processes, and hint at the possibility of prediction, early diagnosis and detection of mutation hotspots.

Bio:

Rudo Roemer is interested in a broad range of topics in condensed matter theory ranging from the mathematical physics of exactly solvable interacting quantum many-body systems to disordered

quantum systems and the applications of computational physics to protein flexibility and dynamics. He uses ideas from the theory of defects in electronic systems to compute the transport and localization properties of charges on short and long DNA strands [Scientific Reports 2, 272-9 (2012), Phys. Rev. Lett. 100, 018105 (2008), Biophys. J. 89, 2187 (2005)]. He is author of more than 160 scientific publications, has given more than 200 talks and conference presentations and organized numerous workshops and conferences. His research experience has spanned three continents (USA 1989–1990, 1992–1994, India 1994–1995, Germany 1996–2002, UK 2002–present) and involves editorial roles for EPL, Scientific Reports and Physica E. He served as Director of Warwick's interdisciplinary Centre for Scientific Computing during 2005-2010."

SPEAKERS: DAY 2

SESSION 3

Photon and electron counting statistics: a tool box for probing quantum effects in biomolecules

Alexandra Olaya-Castro, UCL

It is well known that the primary steps on 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 the formation of such excitons is essential for efficient absorption of sunlight by photosynthetic organisms. 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 or how such quantum features affect the biological function of photosynthetic complexes. In this talk, I will present our research on the quest of signatures of quantum coherent process in photosynthetic complexes with a focus on the fingerprints such phenomena may leave in photon and electron counting statistics experiments. Our work shows that frequency-filtered photon statistics could provide unambiguous signatures of coherent interactions between electronic and vibrational degrees of freedom in light-harvesting complexes and that electric current fluctuations could provide information on the functional role of the vibrational motions assisting energy and charge transfer in photosynthetic reaction centres.

Bio

Alexandra Olaya-Castro received her Ph D in Quantum Physics from the University of Oxford (2005), held a Junior Research Fellowship at Trinity College, Oxford University (2005-2008) and joined the Department of Physics and Astronomy at University College London in 2008 with an EPSRC Career Acceleration Fellowship. She was appointed as Lecturer in 2011 and promoted to Reader (Associate Professor) in 2015. Her research concerns the theory of quantum dissipative dynamics and non-trivial quantum effects in nanoscale molecular systems relevant for biology and chemistry. This research has the potential both to transform our understanding of fundamental processes in biological systems and to provide insight for the development of new quantum-enhanced energy and sensing technologies.

Experimental sequence space exploration of a fitness landscape of short RNA molecules

Jose Jimenez, University of Surrey

The origin of life is believed to have progressed through an RNA world, in which RNA acted as both genetic material and functional molecules. In this prebiotic context, the evolutionary fate of the first functional sequences of RNA would be determined by the structure of the evolutionary fitness landscape of the molecules, which would condition their survival during processes of natural selection. Although fitness landscapes are the subject of much speculation, their structure is essentially unknown. In this work we describe the first comprehensive map of an experimental fitness landscape, exploring nearly all of sequence space, for short RNAs surviving selection in vitro. The landscape was generated synthesizing a library of aptamers of RNA including almost all possible combinations of length 24 with a 1000 times coverage of each unique sequence. The resulting pool of 1017 molecules was subject to screening for binders to GTP attached to a resin. The evolutionary dynamics of the experiment in successive rounds were monitored by deep-sequencing and the biochemical properties of the most relevant hits were characterized. Based on the results obtained

by that approach we estimated the fitness of all sequences surviving the selection and clustered them in families according to their sequence similarity. With the exception of a small evolutionary network, we find that fitness peaks are largely isolated from one another, which highlights, in a 'classical' view of evolution, the importance of historical contingency and indicates that natural selection would be constrained to local exploration of the space of sequences in the RNA world. I will discuss, in light of quantum properties of biological polymers, the possibility of existence of alternative landscapes precluding a higher density of functional sequences in the same pool.

Bio

Jose Jimenez is a molecular microbiologist that earned his Ph.D. in 2006 working for Spanish Research Council (CIB-CSIC) in environmental bacteria for the removal of pollutants. After that he moved into systems and synthetic biology of bacteria in a postdoctoral stay in the National Center for Biotechnology (CSIC; Spain) where he developed molecular tools for engineering metabolic pathways. In 2010 he joined the Center for Systems Biology at Harvard University (USA) as a Fellow for the Foundational Questions in Evolutionary Biology program to study evolutionary dynamics of microbial and prebiotic systems. In 2012 he enrolled in the Synthetic Biology Center at MIT (USA) as a postdoctoral associate where he studied mechanisms of cellular competition for gene expression in bacteria. He has lead the SynBio lab at Surrey since 2014 focusing on the idea of cells as economical system in which the allocation of resources is optimised to maximise fitness.

Environment-Assisted Transport through Single-Molecule Junctions

Jakub K. Sowa[1], Jan A. Mol[1] , G. Andrew D. Briggs[1] , Erik M. Gauger[2]

Single-molecule electronics has been envisioned as the ultimate goal in the miniaturisation of electronic circuits. While the aim of incorporating single-molecule junctions into modern technology still proves elusive, recent developments in this field have begun to enable experimental investigation of fundamental concepts within the area of chemical physics. One such phenomenon is the concept of Environment-Assisted Quantum Transport (ENAQT) which has emerged from the investigation of exciton transport in photosynthetic complexes where it has been suggested that environmental coupling can significantly increase the energy transport efficiency at room temperature in vivo.

I will present results of theoretical studies on charge transport through a two-site molecular junctions coupled to a vibrational environment. The two-site character of the system can be achieved by breaking the conjugation (introducing regions of low π-electron density) within the system, and several structures of this type have recently been investigated in the transport setting. It will be shown that, similarly to what has been suggested in the context of energy transport, vibrational interactions can also significantly enhance the electric current through specific molecular orbitals. I will also demonstrate that in these systems a combination of energetic disorder and environmental coupling can result in current values which exceed what is available from the archetypal idealised quantum channel (noiseless, degenerate wire). This observation goes beyond the typical interpretation of ENAQT of mitigating the effects of energetic disorder. From an experimental perspective, this study offers a clear pathway towards finding and identifying environment-assisted transport phenomena in charge transport settings.

[1]Department of Materials, University of Oxford, Parks Road OX1 3PH Oxford.
[2]SUPA, Institute of Photonics and Quantum Sciences, Heriot-Watt University, EH14 4AS, Edinburg

Towards ab initio Modelling of Quantum Effects in Biology

Daniel Cole, School of Chemistry, Newcastle University

Recent progress in linear-scaling density functional theory (DFT) software allows electronic structure calculations of systems comprising many thousands of atoms to be performed on a routine basis, allowing access to typical length-scales in many biological molecules [1]. I will give two examples from our work in which DFT has played a role in elucidating possible functional roles of quantum effects in biology. In the first example, linear-scaling DFT is used to parameterise a model Hamiltonian to describe energy transfer in the Fenna-Matthews-Olson light-harvesting complex [2], and to reveal the role of correlated static disorder in protecting its ensemble excitonic structure from large thermal fluctuations [3]. In the second example, I will discuss a potential new aspect of quantum biology that has received relatively little attention to date, namely the functional role of quantum many-body effects in transition metal containing proteins [4]. Overall, linear-scaling DFT shows promise as a tool for investigating a range of quantum phenomena in biology.

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[4] Weber C, Cole DJ, O'Regan DD, Payne MC. Renormalization of Myoglobin-ligand Binding Energetics by Quantum Many-body Effects. Proc. Natl. Acad. Sci. USA 2014, 111, 5790-5795.

Memory effects in Open Quantum Systems

Nick Werren, Jim Al-Khalili and Andrea Rocco, University of Surrey

Quantum mechanics is the physical description of matter at a level deeper than we can directly perceive. When a physical object is interacted with by the environment, the wavefunction collapses, the wave-like behaviour ceases and the object behaves classically.

My current project is an investigation into the feasibility of quantum mechanical phenomena being present within a complex biological system in which the environment is constantly interacting with the system. The aim is to construct a theoretical model of a simple system in constant interaction with its own environment can maintain, and then exploit, quantum mechanical behaviour through non-markovian mechanics. This involves modelling the environment as a thermal bath of harmonic oscillators, using Richard Feynman's path integral approach of quantum mechanics, and adjusting certain approximations to gain more insight into such systems.

The advantages of such a project is that it increases the feasibility of the presence of quantum phenomena in biological systems. Such adaptations throw up many more interesting questions within both biology and physics, and any research would necessitate further collaboration between the two disciplines.

Funding Body: STFC, The Department of Microbial Sciences & The Department of Physical Sciences

SESSION 4

Non-optical nanoscale functional imaging for studying ion channels and receptors

Peter Wright and Julia Gorelik, Imperial College London

Conventional physiological techniques for cardiac cells have attained important findings during previous decades. However, few of them resolve physiological processes at the nanoscale level in living cells. Scanning ion conductance microscopy (SICM) is a unique imaging technique that uses similar principles to the atomic force microscope. SICM is a non-optical method which uses a nanopipette as a scanning probe to image the surface topography of living cells and allows one to resolve the structural features of adult rat ventricular cardiomyocytes (ARVMs) such as Z-grooves containing transverse (T) tubules openings and empty crests with a resolution equal to the pipette's inner diameter, typically -30-50 nm. The scanning technique enables simultaneous recording of high-resolution topography of cell surfaces, and cell surface fluorescence. Making it suitable for imaging in combination with Forster Resonance Energy Transfer (FRET) sensor technology (SICM/FRET). The hybrid instrument also functions as a vastly improved patch clamp system (super-resolution scanning patch clamp). The method allows scanning of the surface of living cells noninvasively and enables measurement of cellular activities under more physiological conditions than is possible with other techniques.

As the activity of various receptors and ion channels is highly organized in space and time, it is essential to correlate intracellur signalling with cell structures and subcellular compartments. We describe and validate SICM combined with conventional methods (FRET, patch-clamp, intercellular recording and optical mapping of impulse propagation) as a new technique for cardiac cell physiology. Such hybrid technologies reveal functional localization of different receptors and of ionic currents.

Bio

I began a joint MRes/PhD program in 2009. My PhD project was conducted in Professor Julia Gorelik's laboratory. In the course of this project I investigated subtle differences in the molecular control of the beta-2 adrenergic receptor in different parts of the cardiac muscle, and the possibility of these processes being subverted in disease. My first post-doctoral position, beginning in 2014, was a joint project co-supervised by Julia Gorelik and Professor Cesare Terracciano- at Imperial College. During this time I investigated the mechanosensitivity of molecular mechanisms controlling beta-adrenergic receptors and calcium channels. In the course of both of these projects I have utilized scanning ion conductance microscopy and genetically-encoded FRET biosensors (both separately and in combination). This has allowed me to assess aspects of the control of receptor function within sub-micrometer domains of cardiac cells.