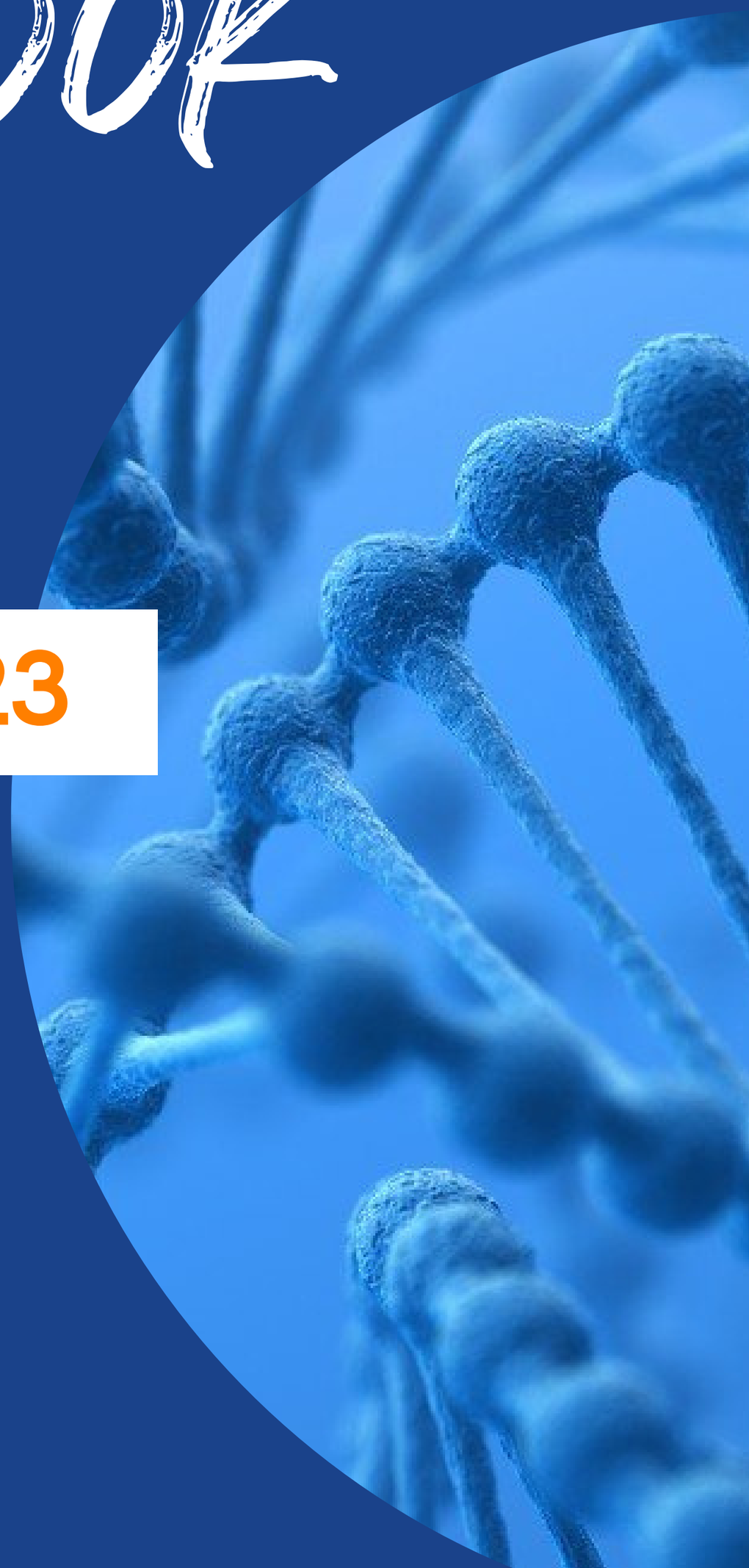
Abstract Book



QuEBS 2023

Quantum Effects in Biological Systems Workshop 2023

26-30 JUNE 2023

QuEBS 2023

UNIVERSITY OF SURREY

Keynote Speakers

2023 QuEBS

Greg Engel

University of Chicago

Quantum Dynamics of Photosynthetic Light Harvesting: Design Principles for Steering and Harvesting Energy

Controling excited state dynamics at the nanometer to micron scale remains a grand challenge for energy science, optical communications, and artificial photosynthesis. Interestingly, it hasn't been a grand challenge for biology for over 2 billion years: nature has already done it. My research group seeks to dissect microscopic mechanisms and quantum dynamics of photosynthetic light harvesting and export these ideas to chemical and material systems. We want to know how photosynthetic antenna complexes collect light and funnel it to the reaction center with near perfect quantum efficiency and exquisite precision. We create new instruments to probe these femtosecond dynamics, and we can use these signals to intuit excitonic transport from the spectral signals. Recently, we acquired data showing a complex interplay between the chlorophyll molecules and their environment within the protein. [1-3] The resonance between delocalized excited states and vibrations on individual chromophores is used to steer excitonic energy toward the reaction center.[1] This approach represents a different approach to dictating energy transfer from what we can create in a beaker. This data has forced us to reconsider the role of a structured environment in energy transfer and continues to fuel the debate on coherent mechanisms of energy transfer in photosynthesis. Moving beyond traditional spectroscopy to gain more direct spatial information, we implemented chiral nonlinear spectroscopy to track wavefunction collapse after excitation to reveal how biology exploits dephasing to efficiently absorb light while systematically frustrating re-emission.[4]

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Alexandra Olaya-Castro

University College London

Towards Probing Quantum Processes in Single Biomolecules on a Chip

abstract

Sharon Hammes-Schiffer

Yale University

Proton-Coupled Electron Transfer in Enzymes and Photoreceptor Proteins

Proton-coupled electron transfer (PCET) reactions play a vital role in a wide range of biological processes. This talk will summarize the main concepts from our PCET theory and will present applications to enzymes and photoreceptor proteins. Our general theoretical formulation for PCET includes the quantum mechanical effects of the electrons and transferring protons, as well as the motions of the donor-acceptor modes and solvent or protein environment. This PCET theory enables the calculation of rate constants and kinetic isotope effects for comparison to experiment and the study of nonequilibrium dynamics. Our application of this theory to PCET in soybean lipoxygenase provides an explanation for the unusually large kinetic isotope effects in terms of hydrogen tunnelling in a constrained enzyme environment. A more recent application explores the PCET pathway for the enzyme ribonucleotide reductase (RNR), which is essential for DNA synthesis and entails six PCET reactions spanning more than 32 Angstroms across an aqueous interface. Our quantum mechanical/molecular mechanical (QM/MM) free energy simulations provide insight into the roles of conformational motions, hydrogen bonding, and proton relays. The final application will focus on blue light using flavin (BLUF) photoreceptor proteins, which are critical for the light regulation of many physiologically important processes. In the Slr1694 BLUF photoreceptor, photoexcitation to a locally excited state within the flavin instigates electron transfer from a tyrosine to the flavin, followed by proton transfer from this tyrosine to the flavin and then a reverse PCET that produces the light-adapted signaling state. Our excited state QM/MM molecular dynamics simulations provide insights into the nonequilibrium dynamics of photoinduced PCET in the BLUF photocycle as well as the nature of the elusive light-adapted state. Overall, our theoretical studies highlight the importance of electronic and nuclear quantum effects, as well as conformational sampling and dynamics, in biological processes.

Sam Hay

University of Manchester

Hydrogen tunnelling and quantised vibrations in enzyme-catalysed reactions

While it is well established that thermally-activated quantum mechanical tunnelling (QMT) of electrons and hydrogen plays a role in many enzyme-catalysed reactions [e.g. 1], there are few definitive experimental signatures of QMT and no clear methods of directly estimating the relative tunnelling contribution from typical experimental data. As most enzyme reactions involve the binding/capture of freely diffusing substrate(s), reactions are typically initiated by mixing and experimental conditions must then be compatible with liquid water. This precludes the classic test of tunnelling: the observation of temperature-independent rate constants at cryogenic temperatures. H-tunnelling is usually inferred from kinetic isotope effects (KIEs) that are larger than the semiclassical limit. Here, we will explore correlations between experimental KIEs, activation free energy terms, and computed tunnelling contributions in order to propose 'signatures' of QMT during enzyme catalysed reactions [2,3]. We will also discuss the role of quantised vibrations and consider experimental probes of their contribution to such reactions.

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Clarice D. Aiello

University of California, Los Angeles

From nanotech to living sensors: unraveling the spin physics of biosensing at the nanoscale

Substantial in *vitro* and physiological experimental results suggest that similar coherent spin physics might underlie phenomena as varied as the biosensing of magnetic fields in animal navigation and the magnetosensitivity of metabolic reactions related to oxidative stress in cells. If this is correct, organisms might behave, for a short time, as “living quantum sensors” and might be studied and controlled using quantum sensing techniques developed for technological sensors. I will outline our approach toward performing coherent quantum measurements and control on proteins, cells and organisms in order to understand how they interact with their environment and how physiology is regulated by such interactions. Can coherent spin physics be established –or refuted! –to account for physiologically relevant biosensing phenomena and be manipulated to technological and therapeutic advantage?

Jonathan Woodward

University of Tokyo

Microspectroscopic detection of magnetic field sensitive radical pair processes in biological systems

In the 1970s, it was established that weak magnetic fields could alter chemical reactions proceeding through the formation of reaction intermediates known as spin-correlated radical pairs. The radical pair mechanism explains this behaviour and reveals how magnetic fields even as weak as the Earth's can measurably affect chemical reaction rates and yields, despite inducing a change in energy of orders of magnitude less than the thermal energy. The radical pair mechanism currently represents the most widely accepted hypothesis to explain the magnetic compass ability of migratory birds [1] as well as magnetoreception in many other animals, and represents a unique example of a biological capability enabled exclusively by virtue of a coherent quantum mechanical process. However, direct evidence for radical pairs undergoing magnetic field sensitive reactions in living systems remains sparse.

Photochemically generated radical pairs and magnetic field effects thereon have been extensively studied experimentally in chemical systems. In order to confirm and fully investigate their role in biology, we have developed microspectroscopic methods based on established spectroscopic techniques to monitor photochemical reactions proceeding through radical pair intermediates with sufficient time resolution, spatial resolution and sensitivity in real time to observe species at cellular level concentrations on submicron length scales. Here I present our studies on radical pairs exploiting both transient optical absorption microscopy and fluorescence microscopy for a wide range of radical pair reaction environments from aqueous solution to living cells. While transient optical absorption methods provide direct spectroscopic and time-resolved information about the radical pairs, fluorescence microscopy provides far less detailed information, but with much greater sensitivity. I will present details on our studies of magnetic field effects on cellular autofluorescence [2] which provide direct evidence for the radical pair mechanism operating in living cells, overview our progress in observing spin effects in single radical pairs [3], and introduce our most recent technique which exploits the combination of a nanosecond, single colour, laser pump-probe method with a rapidly switched magnetic field, allowing direct measurement of radical pair lifetimes with high sensitivity and time resolution and overcoming the disadvantages of conventional fluorescence microscopy.

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Invited Speakers

2023 QuEBS

Richard Cogdell

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Recent Advances in the Understanding of the Structure and Function of Purple Photosynthetic Bacterial LH2 complexes

Photosynthetic light harvesting has been a very active area of research for those interested in quantum effects in biology, for example [1-3]. All these detailed studies have been underpinned by high resolution structural information that has provided three-dimensional visualisation of the arrangement of the pigments and proteins that form the light harvesting complexes [4,5]. The light harvesting complexes from the purple photosynthetic bacteria have been particularly instructive in this regard, since in these species the different pigment groups are spectrally well separated. This makes the functional studies on their energy transfer reactions much more straightforward to understand.

Recently there has been a dramatic increase in the structural information due to the application of single particle Cryo-EM. In this presentation I will describe some of these new structures and show how they now allow us to understand the molecular mechanisms that control both the 'ring size' and the spectroscopic properties of LH2 complexes [6,7].

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Erik Gauger

Heriot-Watt University

Erik Gauger[1], Nick Werren[1], Moritz Cygorek[1], Will Brown[1], Scott Davidson[1], Alexandre Coates[1], Dominic Rouse[2], Stefano Tomasi[3], Ivan Kassal[3], Brendon Lovett[4], Jonathan Keeling[4], and Felix Pollock[5]

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Bio-inspired quantum energy harvesting based on collective light-matter effects

Networks of interacting molecular optical dipoles play an important role in photosynthetic light harvesting, and also hold significant promise for future artificial technologies. In this presentation I will give an overview of our recent theoretical work that takes inspiration from biological structures and processes, with the aim of designing systems that utilise collective quantum optical effects. These enable quantum-enhanced light harvesting [1-2], the charging of a Dicke quantum battery through superabsorption [3], and achieving efficient long-range energy transport (4). I will also briefly introduce recent methodological advances that facilitate the straightforward and numerically exact simulation of complex quantum systems embedded in multiple non-additive environments [5], as is typical of biological and bio-inspired systems.

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Louie Slocombe

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Max Winokan[1], Jim Al-Khalili[2], Marco Sacchi[3]

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Quantum Tunnelling Effects in the Guanine-Thymine Wobble Misincorporation via Tautomerism

DNA polymerase is an enzyme that catalyzes the synthesis of DNA molecules by matching complementary deoxyribonucleoside triphosphates (dNTP) to the template DNA strand using the standard Watson–Crick base pair rules. However, when a noncomplementary dNTP diffuses into the active site during the polymerase dNTP sampling, the polymerase domain will transition from an open to an ajar conformation, thus forming a different nonstandard hydrogen-bonded base-pairing arrangement called wobble mispair [1]. While there are other sources of replication errors, the fidelity of replication primarily depends on the ability of polymerases to select and incorporate the correct complementary base [2].

Consequently, misincorporating a noncomplementary DNA base in the polymerase active site is a critical source of replication errors that can lead to genetic mutations [3]. In this work [4], we model the mechanism of wobble mispairing and the subsequent rate of misincorporation errors by coupling first-principles quantum chemistry calculations to an open quantum systems master equation [5]. This methodology allows us to accurately calculate the proton transfer between bases, allowing the misincorporation and formation of mutagenic tautomeric forms of DNA bases. Our calculated rates of genetic error formation are in excellent agreement with experimental observations in DNA. Furthermore, our quantum mechanics/molecular mechanics model predicts the existence of a short-lived “tunnelling-ready” configuration along the wobble reaction pathway in the polymerase active site, dramatically increasing the rate of proton transfer by a hundredfold, demonstrating that quantum tunnelling plays a critical role in determining the transcription error frequency of the polymerase.

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Nirosha Murugan

Department of Health Sciences, Wilfrid Laurier University, Waterloo, ON, Canada

Harnessing biophysical communication to instruct cell fate and control disease

Biophysical communication is a powerful determinant of tissue patterning that is intrinsic to embryonic development, limb regeneration, and cancer proliferation. Parallel to the molecular gradients and transcriptional networks that orchestrate cellular organization, the evidence suggests that cell fate and behaviour can be programmed by mechanical, electrical, magnetic, and optical signalling. Because biophysical signals are emitted endogenously or embedded as cues within tissue microenvironments, we have developed novel tools and techniques to non-invasively and precisely detect pathologies. Indeed, we can now “read” the biophysical states of diseased cells and tissues by detecting their ultraweak photon emissions (UPEs) in real-time with fingerprint-like spectral profiles that are readily distinguished from healthy counterparts. In a recent set of experiments, we demonstrated that brain derived UPEs predicted neural activations associated with sensory inputs and neurocognitive tasks. Similar assessments can be performed by characterizing the stiffness of the extracellular matrix (ECM) or the electrical dynamics of resting membrane potentials (V_{mem}). Interestingly, applied light, electromagnetic fields (EMS), and mechanical forces can also be used to “re-write” biophysical states. Our laboratory has focused on inhibiting cancer cells by interfering with endogenous biophysical communication. For example, we have used weak electromagnetic fields to inhibit melanoma tumour growth in a rodent model. Together, these findings suggest that biophysical communication is both fundamental to the functions of cells and potentially exploitable as a means of “reading” and “writing” cell fates toward novel anti-cancer therapies. Equipped with the means of programming or re-programming tissues, exploiting biophysical states towards developing diagnostic tools will improve the early detection and intervention of many pathological conditions.

Carlos Martino

Johns Hopkins University

Nam Le[1], Michael Salerno[1], Ryan McQuillen[1], Megan Hannigan[1]
Johns Hopkins University - Applied Physics Laboratory 11100 Johns Hopkins Road, Laurel, MD 20723, USA

The Quantum Biology of Reactive Oxygen Species Production in Electron Transfer Flavoprotein

We propose a novel domain within quantum biology: control of the biological production of reactive oxygen species (ROS) by influencing spin dynamics in a radical pair (RP) reaction. Our exemplar system is the human electron transfer flavoprotein (ETF), which is biologically critical for ROS regulation with impacts on stress, cognition, and aging. We test the hypotheses that the flavin:superoxide [$FADH^{\bullet}$… $O_2^{\bullet-}$] RP plays a key role in the partitioning of ROS products from ETF, and furthermore that the partitioning can be affected by external fields.

We show evidence that $O_2^{\bullet-}$ could meet strict constraints for possible involvement in magnetic field effects in the system $FADH^{\bullet}$… $O_2^{\bullet-}$. The main constraint set forth previously is that the fast spin relaxation of $O_2^{\bullet-}$, if unimpeded, would lead to RP coherence lifetimes too short to be influenced by external fields. To that end, we have recent evidence that $O_2^{\bullet-}$can bind tightly to certain sites in ETF and be stabilized by nearby charged protein residues. Our recent relevant findings are summarized here and published. Moreover, theoretical calculations indicate that nuclear spin (i.e., hyperfine) interactions in the flavin and $O_2^{\bullet-}$ system are highly anisotropic, and thus potentially susceptible to external field effects. In coupled experiments, we have purified ETF and begun to characterize preliminary magnetic field effects on ROS production.

We test and exploit the anisotropic hyperfine centers of the flavin:superoxide RP system in ETF to maximize coherent lifetimes, which will result in higher magnetic sensitivity. Guided by our published and preliminary work, we use point mutations near the binding site, as well as external magnetic fields, to enhance coherent lifetimes. A chip-based optical platform is developed to exploit the anisotropy of the system by anchoring oriented protein molecules and varying the angle of the external magnetic fields.

Alex Jones

National Physics Laboratory

Alex R. Jones[1], Adam A. Bradlaugh[2], Giorgio Fedele[3,4], Anna L. Munro[2], Celia Napier Hansen[3], John M. Hares[3,5], Sanjai Patel[6], Charalambos P. Kyriacou[3], Ezio Rosato[3], and Richard A. Baines[2]

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Essential molecular elements for magnetosensitivity in Drosophila

It has been estimated that the Earth's magnetic field (geoMF) contains 5 to 6 orders of magnitude less energy than the thermal energy, k_BT, of a typical biological system. Yet somehow certain animals have evolved to sense the geoMF through this thermal noise to help them navigate their environment. Biochemical reactions that proceed *via* radical pair intermediates that transiently adopt spin polarised states are uniquely placed to provide a means by which a biological system might be able to sense and transduce a magnetic signal. Such intermediates have been identified in light-sensitive versions of the signalling protein, cryptochrome.

The fruit fly, *Drosophila melanogaster*, has a magnetic sense and serves as an ideal, genetically-tractable *in vivo* system with which to investigate the molecular machinery required for an animal to perceive weak MFs [1]. The magnetic sense of *Drosophila* appears to be dependent on light and the presence of cryptochrome. I will present data from single cell electrophysiology measurements [2, 3] and whole organism behaviour assays [4] that reveal what could be the essential molecular elements of magnetosensory perception and signal transduction in *Drosophila* [5]. These data provide insights into the possible evolutionary origins of cryptochrome-dependent magnetoreception and suggest that similar mechanisms for magnetic perception might occur in both migratory and non-migratory animals.

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Thorsten Ritz

University of Calafornia

Shawn Strausser[1], Phillise Todd[1], and Maria Procopio[1]

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Quantum Sensing with Fast Biological Signal Transduction

For more than 20 years, Cryptochromes (CRY) employing the radical-pair mechanism for detection of weak magnetic fields, has been the leading candidate for a biological quantum sensor. Most attention has been focused on how a single reaction step, usually in the light-activated reduction of CRY can be influenced by a magnetic field. This exclusive focus has precluded addressing even very basic questions about the postulated quantum sensor, the signal-to-noise ratio, bandwidth, and the time required to obtain a readout.

Here, I will argue that a CRY-based quantum sensor not only can operate at low-light intensities, such as during dusk or at night in nature, but will operate optimally under low-light conditions, potentially giving a reason why birds fly at night. This optimal window at low light-intensities sets strong constraints on the rate of CRY activation, which in turn makes virtually every CRY sensor discussed to date a very slow sensor with readout times on the order of tens of hours. Clearly this is at odds with experimental evidence of bird magnetic orientation which indicate an orientation decision within at most minutes. This large time-scale gap appears to be the most fundamental objection to the idea that CRY and the radical-pair mechanism underlie magnetic sensing in biology. I will discuss three possibilities of how the signal transduction from CRY might be sped up with the hope of triggering more research into this aspect of quantum biological sensing.

Luca Sapienza

University of Cambridge

Bio-molecules on a chip: implementing nano-fabrication technology to investigate photosynthetic light harvesters

I will present our research work that aims at isolating single light-harvesting complexes on a chip, in particular through the implementation of a photo-luminescence imaging technique that we have developed [1].

I will show preliminary results on the investigation of the emission properties of biomolecules by means of micro-photoluminescence spectroscopy, under continuous-wave and picosecond-pulsed laser excitation, down to cryogenic temperatures, measurements aimed at understanding recombination mechanisms in photosynthetic complexes.

I will then discuss nano-fabricated photonic devices [2, 3, 4] that can be implemented in order to increase the light-matter interaction in biomolecule-optical cavity coupled systems, and maximise the collection efficiency. The latter is particularly important to carry out photon correlation measurements that can unveil the role of quantum effects in the way biomolecules function [5].

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Short Talks

2023 QuEBS

Alasdair Mackenzie

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Alasdair M. Mackenzie[1], Holly E. Smith[1], Rhys R. Mould[2], Geoffrey W. Guy[3], Alistair V.W. Nunn[2,3], Jimmy D. Bell[2], and Stan W. Botchway[1]

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Biology in the dark: Investigating single photon emission from growing mung beans

Ultraweak photon emission (UPE) in the range of 10-100 photons/s/cm2 has been reported from many different cell types. The source of this light is thought to be from the decay of reactive oxidative species possibly from inside the mitochondria, chloroplasts and bacteria. It is suggested that UPE may be used for intra and inter cell-cell photonic communication and have implications on the origin of life.

Studies on this light emission were undertaken on growing mung beans. Apparatus design and considerations when working with ultra-weak light are discussed. Investigations into these UPE were performed using a dual opposing photomultiplier tubes setup on imbibed beans over 7 days. At constant temperature (21 + 1 oC), we show that beans grown from seeds generated emission of 5 + 1 photons per second. As the new bean stems increase in size they show gradual increase in emission up to 30 + 1 photons/s. Actively growing seeds also showed episodic bursts of emission lasting around an hour before returning to their previous levels. The bursts of emissions do not correspond to day and night cycles as would be expected.

Interestingly UPE was strongest underneath the growing beans, indicating emission mostly from roots. The bursts of photons also correlated well with increased secondary root growth. Using H2O2 (0.167 µM) which promotes secondary root growth, we observed a significant increase in photon emission compared to water alone. Altogether, we demonstrate a clear and significant correlation between an increase in UPE with plant secondary root growth. Using our set up, we are able to separate UPE originating from the plant roots and from leaves where chlorophyll emission may dominate. We speculate that the low level of UPE detected may have implications for quantum effects of single photons on plant growth and function. These speculations will form part of our future studies on live plant and mammalian cells.

Anna Munro

The University of Manchester

Adam Bradlaugh[1], Richard Baines[1], and Alex Jones[2]

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Drosophila Cryptochrome: signalling the effects of a magnetic field to a neuron.

It is well documented that Cryptochrome, or at least its C-terminus, is sufficient to mediate magnetic field sensitivity in a blue light dependent manner via the radical pair mechanism. The signalling of these effects however is much more poorly understood, particularly those on membrane excitability of Drosophila neurons. The current model suggests that magnetic field effects on neuronal activity are a potentiation of blue light induced changes in cellular redox, increasing excitability through changes in the redox state of the cell which affect ion channel conductance. However, recent data from our lab implicates the importance of the interaction domains in the C-terminus of DmCRY in signalling magnetic field, but not blue light, effects. Moreover, several mutations/treatments reveal interesting insights into the possibility of separable signalling pathways of CRY dependent blue-light and blue-light dependent magnetic field effects.

Avi Schneider

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Spin Exchange Interaction and Protein Structural Stability

The abundance,and enantiomeric purity, of chiral molecules and structures in biological systems raises a question of the role chirality plays in biology and provokes thoughts on the evolutionary pathways that brought forth the fixation of such an asymmetric dominance.It has been found that chiral molecules possessuniqueintrinsic traits relating tothe fundamental quantum-mechanical property of electron spin. This phenomenon, termed Chiral Induced Spin Selectivity (CISS), influences the distribution, transmission and scattering of electrons through chiral molecules, based on compatibility between the electron spin state and the handedness of the molecule. With these concepts in mind, we set out to experimentally investigate the involvement and importance of electron spin in functioning biological systems such as enzymatic catalysis and protein folding.Using various detection methods, we assess the structural integrity of proteins under increasing denaturing conditions, while comparing the influence of surface-magnetization-controlledspinexchange interactions on the denaturation trend of the proteins.The results fromour previous and present research indicate clear correlations between the electron spin distribution in a protein and its structural stability [1]. We hypothesize the involvement of intrapeptide spin exchange interactions inthe determination and preservation of protein structure, in addition to well-established and accepted contributing factors. Our findings motivate us to further uncover the widely overlooked, potentially pivotal, underlaying role of electron spin in biological systems.

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Catxere Casacio

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Towards coherent dynamics of fluorescent proteins with DNA origami

Understanding the mechanisms of life and ultimately what is life is a challenge that many scholars from different backgrounds have pursued throughout human history. The interdisciplinary field of quantum biology is paving the way to describe life at atomic levels. In particular, the process of Förster resonance energy transfer (FRET) between fluorophores is intensively used to determine structures, dynamics and distances of biological systems. Despite being a powerful tool, basic knowledge on FRET standards is currently only approximative.

Here we show experimental progress to advance fundamental understanding of how the dynamics of energetic processes happen in the excited states of bio-molecular systems. By employing genetic engineering, we modify green fluorescent proteins to allow their conjugation to specific and methodically longer sizes of DNA oligomers, using techniques of DNA scaffolds. Using time-resolved fluorescence spectroscopy, our method allows precise knowledge of distance between the proteins, enhancing our understanding of the system dynamics. From that, we envisage to study through a transient absorption spectroscopic system how the excited quantum states result in coherent energy transfer being maintained in fluorescent proteins under physiological conditions.

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Witnessing coherent quantum transport with two-colour photon correlations

Photosynthetic light harvesting complexes fulfil the biological function of directing energy from sunlight in the form of excitonic excitations towards a reaction coordinate. This transport process is highly efficient, and it is understood that both coherent and incoherent environmental processes can in fact contribute to increasing this efficiency. Exciton transport has an inherent directionality enabling biological function that is induced by environmental processes and characterised the violation quantum detailed balance (QDB). We study a prototype photosynthetic dimer model, and observe that the way in which QDB is violated differs between the incoherent and coherent environmental processes, with increased contribution from the coherent process aiding faster transport, but reducing directional bias. We thus observe a balance between coherent and incoherent processes maximises directional flow over the short timescales involved in exciton transport with biologically relevant conditions. We finally show that the QDB violation, whilst not directly observable in itself for such emitters, may be witnessed through the time-asymmetry of two-colour photon correlations, and that these observable correlations are extremely sensitive to the vibrational mode coupling and resonance to exciton energy gaps, yielding a potential route to experimental verification in realistic molecular system.

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Simulating exciton transport with quantum computers

Just as some biologically relevant processes may exploit quantum coherence for their functioning, in quantum computing we harness the same quantum resource for computational purposes. However, differently from (ideal) quantum computers, which can only implement unitary (time-reversible) operations and measurements, physical systems of bio-chemical interest are rarely isolated and the description of molecular processes requires to take into account the interaction with their environment. It therefore comes naturally to ask whether quantum computers can be used for the simulation of these open systems and which strategies can be devised to account for such non-unitary (time-irreversible) dynamics.

In our contribution, we will elaborate on the opportunity of using digital quantum computers for the simulation of environment-assisted quantum transport (ENAQT) of excitons in chromophore networks, which arises from the interplay between the system electronic Hamiltonian and decoherences due to the interaction with the (vibrational) environment. ENAQT is believed to play a primary role in the high efficiency of natural light-harvesting complexes and its understanding can be useful, for example, for the design of artificial photovoltaic devices. In particular, we will examine some of the best-known methods for describing ENAQT in the Markovian and non-Markovian regime and consider their implementations in terms of quantum circuits based on stochastic trajectories and collision models. We will show that both algorithms can be intended as different unravellings of the same target dynamics. Finally, we will give some perspective on how to simulate the spectroscopic response of chromophore systems using quantum computers.

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Bio-Inspired Chromophore-Protein Assemblies for Solar-Energy Conversion

Oxygenic photosynthesis enables the efficient conversion of solar energy into chemical energy. This complex process starts with the absorption of sunlight by the light harvesting complexes, which subsequently transfer the excitation energy to the reaction centers where charge separation occurs.In this work, we aim to rationally design artificial systems capable of mimicking the properties of natural photosynthetic complexes. For that purpose, zinc-pheophorbide-a derivatives are employed as pigments, whereas different de novo designed four α-helix bundle proteins are used as matrix. The excited state dynamics of the artificial systems has been tracked by means of two-dimensional electronic spectroscopy and transient absorption techniques. Moreover, circular dichroism has been employed to confirm the excitonic interactions present in the chromophore-protein assemblies. The recorded data evidence novel operative relaxation channels when chromophore dimers are inside the protein matrix, which are investigated in terms of their dependence on vibronic coherence.

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Protection of Quantum Coherence by Optimizing Network Geometry

We investigate how the geometry of buffer networks impacts the protection of quantum coherence in spin clusters that interact with thermal environments. We explore all buffer networks that can be embedded in a plane and find that the connectivity of the buffer network is crucial in determining the protection time of quantum coherence in a single central spin. Our results indicate that the maximal planar graph provides the longest protection time for a fixed number of buffer spins. However, increasing the number of buffer spins does not always lead to longer protection times [1]. With the help of a quantum master equation [2], our simulations show that a tetrahedral geometry of a four-spin buffer network offers the most optimal protection against environmental effects. These findings could help us to better understand biochemical processes since we frequently observe tetrahedral geometry in natural molecules [3].

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BioCrystallography: Structural proteomic biomarkers for early non-invasive diagnostics

An extracellular matrix (ECM) is a dynamic three-dimensional network of macromolecules that provides structural and functional support for the cells. ECM plays critical regulatory roles in morphogenesis since it orchestrates cell signaling, functions, properties, and morphology. The ECM structure is constantly being remodeled and altered as a response to various external and internal factors. Moreover, we can see it as a global transcription of local morphogenesis events. In this sense, structural analysis of the ECM can reveal many pathologies non-invasively. A standard procedure of usual crystallography –X-ray diffraction –can monitor the status of periodic components of ECM, such as lipids, glycoproteins, collagen, and keratin. The high sensitivity of this method allows the detection of subtle changes in the structure and facilitates the early diagnostics and screening of pathological alterations in Structural Proteomics Biomarkers(SPB). For the proof of principles, we studied the keratin samples taken from the claws of the dogs with and without developed cancer. X-ray diffraction patterns demonstrate the striking difference between healthy and cancerous samples. In particular, one of SPB, a feature responsible for the keratin dimers separation in the filament, can be seen in the healthy samples but almost completely disappears in the cancerous ones.

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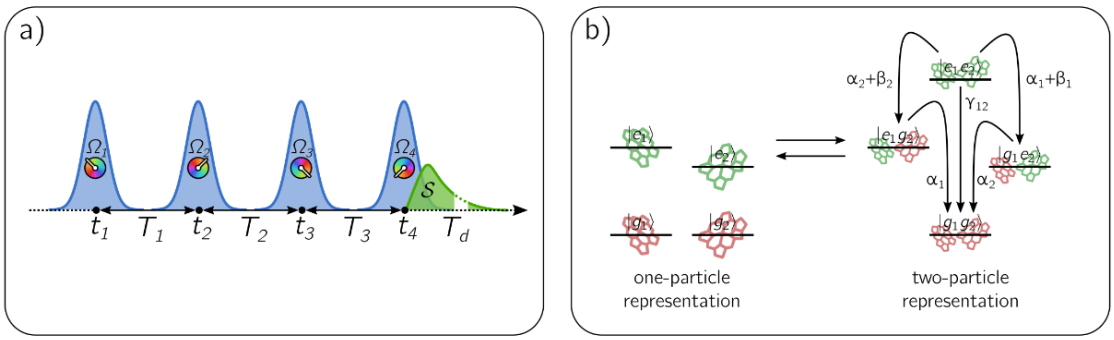
Reconciling Non-Linear Response and Incoherent Mixing in Action-2D Electronic Spectroscopy: from Molecular Dimers to Photosynthetic Systems

Action-2D Electronic Spectroscopy is emerging as a powerful technique to probe exciton and charge transfer processes in photosynthetic complexes and nanostructures. While highlighting the coherent dynamics induced by the interaction with four laser pulses, action detection relies on measuring an incoherent signal proportional to excited-state populations (Fig. 1a), i.e., fluorescence [1] or photocurrent [2], paving the way for the study of systems in vivo [3] and *operando* [4] conditions. Despite its advantages, the origin of certain spectral featuresstill remains ambiguous, i.e., cross peaks at early waiting-time [5] and incoherent mixing [6] contributions, calling for the aid of numerical simulations. To this aim, we set up and test a numerical protocol to simulate the action response of weakly-interactingchromophores using a non-perturbative treatment of the light-matter interaction [7]. Starting from a moleculardimer, we establish the correspondence between the optical response and a kinetic scheme for populations inthe one- and two-particle representations (Fig. 1b) [8]. On this basis, we propose a unified framework thatreconciles incoherent mixing with the theory of non-linear optical response in the presence of exciton-excitonannihilation or other non-linear population dynamics. Finally, we address the scaling of incoherent mixing withthe system size, pointing out how these contributions may completely hide coherent features in the case oflarge photosynthetic systems. Figure 1: a) Pictorial representation of the experiment showing a train of four laser pulses (blue) and the emitted incoherent signal (green). b) One- and two-particle representation of a molecular dimer.



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PcrA helicase protects against quantum mutations

Proton transfer between the DNA bases can lead to non-standard, potentially mutagenic tautomeric forms [1, 2]. Suppose the tautomers successfully pass through the replication machinery. In that case, they are thought to adopt a Watson-Crick-like shape and mismatch with the wrong base, thus evading proofreading and potentially leading to replication error [3]. There is heated debate over the true biological impact of the tautomeric forms. Previously it was proposed that if the tautomeric lifetime is much shorter than the helicase cleavage time, no tautomeric population would successfully pass the enzyme [4]. In our previous work, we have determined that the proton transfer energy landscape drastically changes during the first two Angstrom cleavage of the base and indicate that cleavage time is much quicker than previously thought [5]. These results suggest that a static picture of the proton transfer oversimplifies the biological event.

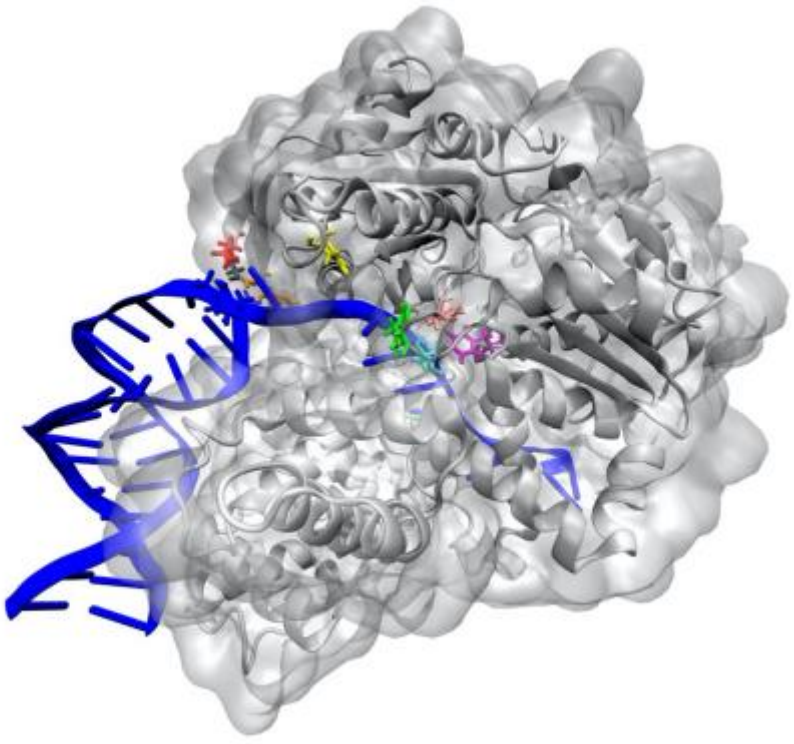

Figure 1: DNA bound to the helicase enzyme. One DNA strand can be seen being pulled through the enzyme. While key residues in the helicase are highlighted.

PcrA helicase (Figure 1) has been well studied in terms of its stepping motor action dynamics [6, 7] and individual amino acid roles in unwinding DNA[8]. Thus PcrA Helicase provides an ideal scenario within which to consider the stability of the tautomeric G*-C* pairing. To further elucidate the complicated environment in which tautomers may be formed, and the dynamics in which they must survive, we employ multiscale quantum mechanics / molecular mechanics (QM/MM) calculations which marry the accuracy of DFT with the large-scale dynamics of MD. The tautomerisation reaction is mapped using Umbrella Sampling to obtain a potential of mean force for DNA in complex with PcrA Helicase for the first time. Understanding the role of the local amino acids at the DNA binding site of this replisome enzyme sheds new light on the feasibility of Löwdin's hypothesis inside a realistic biological environment. We find that the presence of the helicase, radically destabilises the mutagenic conformations, indicating that it is the first line of defence against spontaneous mutation.

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Optical Ratcheting: Bio-Inspired Solar Technology

Quantum physics will undoubtedly play a key role in the development of future solar technologies. This becomes most obvious when we consider the conventional silicon solar cell which faces substantial energy loss through inefficiency, e.g., through conversion of light energy to heat and loss via reradiation. This particular obstacle is wholly captured by the Shockley-Queisser limit. In this talk, we will investigate the potential to overcome this limit by combining an open quantum systems approach with nanoscale structures inspired by the porphyrin ring systems that are known to be pivotal in photosynthesis. Specifically, we demonstrate a mechanism unique to quantum mechanics known as optical ratcheting. We present ratcheting in a number of different contexts, from a naïve and “artificial” regime in which the ring systems are weakly coupled to a vibrational environment to a more physically realistic and appropriate model captured by the polaron frame. In each case, ratcheting showcases the substantial efficiency increases quantum physics can provide existing solar technologies.

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QM benchmark study of the C=C dimer and modelling of a (6,4)T-T Photolyase.

DFT and TD-DFT are commonly used to model DNA lesions, including the cytosine cyclobutane pyrimidine (C=C) dimer. The basis set and diffuse functions chosen can have a large, but sometimes predictable impact on the predicted geometry, thermodynamics and excited state energetics of the lesion. Using the codes Guassian and NWChem, a study was conducted to compare B3LYP and CAM-B3LYP, and Pople and correlation-consistent basis sets to ccsd/eom-ccsd when used to model the C=C dimer. Various charges, solvation and spin states were considered. It is hoped that this will provide a reference guide for future gas-state and solvated C=C dimer studies. A separate AMBER MM and QM/MM study examines the ground state dynamics of a (6,4) Photolyase variant, taken from a file created throughX-ray crystallography1bound to (6,4) thymine (T-T) photoproduct.

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Energy and Charge Dynamics in the Photosystem II Reaction Center

The reaction centres of the photosynthetic protein complexes are where Nature converts solar energy to electricity. We study the reaction centre of photosystem II of green plants. We have calculated the excitation energies and excitonic couplings of the reaction centre using the multiconfiguration method RASSCF/RASPT2. The excitation energies of the chlorophyll molecules are surprisingly asymmetric. We discuss the possible implications of this asymmetry and present preliminary simulations of the energy dynamics in the reaction centre.

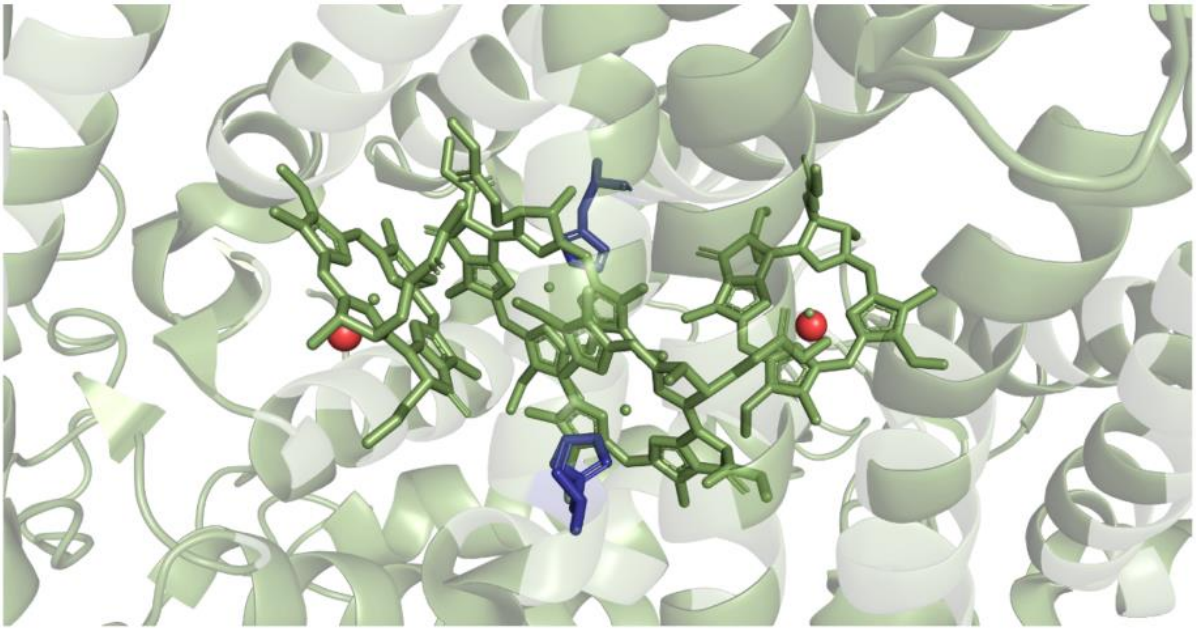

Fig. 1 The Reaction Center of Photosystem II. It appears symmetric at first glance, yet the energetics is not symmetric.

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Interplay of quantum coherence and chiral-induced spin selectivity (CISS) effect in the radical pair mechanism of avian magnetoreception

This work examines the role of chiral-induced spin selectivity (CISS) effect in the radical pair (RP)mechanism of avian magnetoreception [1, 2]. We analyze the impact of spin selectivity (due to CISS) on the sensitivity of the avian compass while considering the dipolar and exchange interactions and their interplay with CISS. We find that CISS significantly increases the compass sensitivity and counteracts the negative effect of dipolar interaction on system sensitivity [1]. The study also explores the effect of spin decoherence on the system and reveals that CISS shows increased compass sensitivity under decoherence compared to the no CISS case. We have also investigated the effect of CISS on quantum coherence in the RP mechanism of avian magnetoreception [3]. We examine the correlation between global and local coherence measures and the yield of the signalling state in the RP model [4]. Our study finds that CISS increases both the relative entropy of global coherence and local coherence in the radical pair [3]. However, only global coherence exhibits a strong correlation with the signalling state yield, indicating a potential utility for the avian compass. Additionally, we analyze the effect of environmental decoherence along with CISS and conclude that a high CISS results in a high correlation of global coherence with signaling state yield despite environmental decoherence. Overall, the study highlights the significant role of CISS in the radical pair model of avian magnetoreception and proposes its potential use in developing quantum technologies by sustaining coherence in radical pair-like quantum systems.

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Spin Fano Resonances in Chiral Molecules

Experiments on spin transport through a chiral molecule demonstrated the attainment of significant spin polarization, demanding a theoretical explanation. We report the emergence of spin Fano resonances as a mechanism in the chiral-induced spin-selectivity (CISS) effect associated with transport through a chiral polyacetylene molecule. Initializing electrons through optical excitation, we derive the Fano resonance formula for the spin polarization. Computations reveal that quasi-degeneracy is common in this complex molecular system. A remarkable phenomenon is the generation of pronounced spin Fano resonances due to the contributions of two near-degeneracy states. We also find that the Fano resonance width increases linearly with the coupling strength between the molecule and the lead. Our findings provide another mechanism to explain the experimental observations and lead to new insights into the role of the CISS effect in complex molecules from the perspective of transport and spin polarization resonance, paving the way for chiral molecule-based spintronics applications.

Main reference:

C.-Z. Wang, V. Mujica, and Y.-C. Lai, “Spin Fano resonances in chiral molecules: An alternative mechanism for the CISS effect and experimental implications,” Nano Letters 21, 10423-10430 (2021).

Poster Presentations

2023 QuEBS

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Allotment Inspired Vision Restoration: use of natural dyes for photosensitive organic semiconductor devices towards retinal implants.

Vision loss due to the degeneration of photoreceptor cells in the retina occurs in millions of people every year worldwide through diseases such as retinitis pigmentosa and age-related macular degeneration. The development of a photosensitive organic semiconductor device that can be implanted and function in a way to replace lost or damaged photoreceptor cells may be a possible treatment for those suffering with these diseases. There are two possible locations for a retinal implant: subretinal (on top of the retina) and epiretinal (in the space between bipolar cells and pigment epithelium). Devices currently commercially available consist of a device implanted epiretinally with images captured by a camera and transmitted to the implant which goes on to stimulate ganglion cells into producing a monochromatic image. We propose a device that can be implanted subretinally and will be self-sufficient, responding directly to photons entering the eye. We hope it will return full colour vision to recipients which is a vital step to restoring quality of life to those with vision loss.

We demonstrate that natural dyes extracted from various berries and vegetables, such as raspberry and beetroot, are excellent chromophore candidates for colour-specific organic devices with similar absorption spectra to those produced by human rod and cone cells. Using fabrication methods resembling those used in the development of dye-sensitised solar cells, bio-derived chromophores have been investigated when bound to a TiO¬2 nanoparticle layer which serves as an electron-collecting electrode. The production of active devices interfaced with electrolyte, phosphate buffered silane, have been demonstrated. Devices produce photocurrent and photovoltage spectra in different spectral regions corresponding to the activity of human cone and rod cells. Our results show the chromophores can respond to pulsed light in a similar way to photoreceptor cells and produce a rising photovoltage.

In summary, we discuss if natural dyes can be used to sensitise a device that can replace degenerated photoreceptor cells and produce a photovoltage capable of stimulating neuronal circuitry in the human eye. We envision a development of technology where pixelated devices can be produced on flexible substrates using printed electronics approaches to be fully compatible with human tissues and working in biological electrolyte environments. We hope this technology will allow for advances in understanding mechanisms behind the efficiency of light detection in the retina.

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eGFP: Influence of dimerization in protonated chromophore stability

Green fluorescent proteins (GFPs) have been extensively studied due to their unique fluorescence properties, making them invaluable tools in various scientific disciplines. This study focuses on the dimerization behaviour of GFPs and its influence on the stability of the protonated chromophore. The protonation states of the GFP chromophore play a crucial role in determining its fluorescence properties. Understanding the different protonation states, including neutral and deprotonated forms, is vital for deciphering the underlying mechanisms of GFP fluorescence. Despite extensive research, the biological significance of GFP dimerization and coherent energy transfer mechanisms remains elusive. However, our findings reveal a protective role of dimerization, suggesting that it may contribute to the stability and functionality of GFPs. We demonstrate that dissociation of the GFP dimer affects the protonation state of the chromophore, highlighting the intimate relationship between dimerization and chromophore stability. Moreover, dimerization enhances GFP's resistance to environmental pH changes, making it more robust under varying conditions. These results provide valuable insights into the role of dimerization in GFPs and have broader implications in understanding protein-protein interactions and the influence of environmental factors on fluorescence phenomena. Computational studies can further elucidate the specific mechanisms underlying pH sensitivity and chromophore-chromophore interaction and aid in unravelling the biological functions of GFPs. These insights can contribute to our understanding of dimerization-mediated phenomena and guide future experimental investigations, ultimately leading to a comprehensive understanding of GFP's biological role and expanding its potential applications in diverse scientific fields.

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Quantum Aspects of DNA Replication and Spontaneous Mutagenesis

The task of DNA replication is central and essential for all known living organisms. There are many environmental factors that can induce mutations during replication, yet a more subtle mechanism that relies only on the intrinsic properties of DNA was proposed by Watson and Crick. In their seminal 1953 paper describing the double helix, they hypothesised that spontaneous mutations could arise when DNA bases adopt rare and energetically less favourable tautomeric forms. Since tautomerisation involves the relocation of protons, the transition could be facilitated by quantum tunnelling. To test this hypothesis, we have employed advanced molecular biology techniques and the single-nucleotide primer extension assay to explore the impact of heavy water (D2O) on the mutation rate, mutation spectrum and misincorporation frequency. Our promising results will be presented.

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Tautomerisation Mechanisms in the Adenine-ThymineNucleobase Pair during DNA Strand Separation

The conclusions of several investigations studying DNA base pair tautomers determine that the energetic stability of the guanine-cytosine tautomeric base pair (G*-C*) is more significant than in the adenine-thymine tautomeric base pair (A*-T*). However, these studies have omitted the dynamics of the DNA strands constructing the double helix implicit to the process of DNA replication. Using density functional theory (DFT), we observe that these dynamics stabilise the A*-T* state to such an extent that the reverse reaction barrier of base pair tautomerisation as a function of strand separation is highly comparable for both the A-T tautomerisation and G-Ctautomerisation reactions. Additionally, using molecular dynamics (MD) we determine that the speed of DNA strand separation is much quicker than previously thought in literature, meaning that the lifetime required of the tautomer to stand a chance of relevance in spontaneous mutagenesis is much reduced. We conclude that the tautomerisation of adenine-thymine is a genuine candidate to be considered as a genetic mutation mechanism in the regime of DNA strand separation.

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Investigation of Heavy Water Effect on Ion Selectivity in ASIC1

Acid Sensing Ion Channels (ASICs) are proton-gated ion channels selective to cations with a higher selectivity toward sodium(Na+) compared to the other cations. They are involved in several important physiological roles[1-2]; hence they are one of the most studied channels of the Epithelial Sodium Channel/Degenerin (ENaC/DEG) superfamily. The ASIC1 subunit can function as a homotrimeric channel and its structure is currently the most established of the whole ENaC/DEG family[2-6]. By computing the single ion free energy profile on different ASIC1 structures, we recently showed that the channel is indeed cation-selective and that the histidine of the conserved 'HG' motif from the re-entrant loop plays an important role for binding Na+[7]. Based on these results and some experiments, we investigated ion selectivity by computing free energy profiles of single ion permeation for other cations(K+and Li+) as well as computing the binding energy using Free Energy Perturbation (FEP). Finally, because the permeating cations are partially hydrated in the selectivity filter, we investigated the effect of heavy water using the TIP3-HW model[8]. Our results suggest that changing the water model to a heavy water one induces changes in free energy barriers and binding free energies, especially for Na+. These results match our experimental results and highlight the significant role of the water shell surrounding the cation for ion permeability and selectivity.

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Identification of Potential Isoniazid Activation Pathway via Molecular Modelling

The activation of isoniazid is an open problem that is becoming increasingly important with the growing prevalence of multi-drug resistance in Mycobacterium tuberculosis (TB). Annually, TB is responsible for 1-2 million deaths worldwide; in 2022 it was reported as 'the second leading infectious killer and the 13th leading cause of death globally' [1] and exists in about one-third of the world's population. HIV sufferers are 15-21 times more likely to develop active TB and the two illnesses form a lethal synergy.

Current TB treatment involves a combination of pharmaceuticals including isoniazid. The exact activation mechanism of isoniazid is undetermined with various candidates available, if we are to combat the increasing incidence of multi-drug resistance in TB we need to first understand how existing antitubercular agents act. In this study we are particularly interested in one such variant, the S315T KatG mutant.

Here we use techniques from across computational and theoretical chemistry and physics to identify a quantum mechanically underpinned mechanism of action for the activation of this antitubercular agent. The base model is the radical pair mechanism [2] adapted to reproduce the results of Timmins [3] which indicate that the activation may be a spin chemical interaction due to the formation of radicals. This particular work is interested in the molecular modelling, that is, use of atomistic techniques to attempt to identify the molecular pathway in the first step of isoniazid's activation.

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Photosynthetic energy transfer dynamics in different environments

The fundamental early steps of photosynthesis are carried out by a network of light harvesting protein-pigment complexes. In photosynthetic purple bacteria, these complexes are embedded in the cell membrane. The lipid composition of the membrane affects the clustering of these complexes and consequently energy transfer between them. Studies of isolated complexes have provided us with an insight into their structure and function, However, the question remains as to the structural and functional impact of isolating such complexes from their physiological environment. Recent studies comparing detergent isolated complexes to membrane embedded complexes have uncovered differences in the complexes spectra and intracomplex energy transfer rates. To address the role of the membrane in intracomplex energy transfer, We compare two models of the peripheral light harvesting complex 2 (LH2) from purple bacteria Rhodoblastus acidophilus, one describing LH2 in the membrane and the other describing detergent isolated LH2. We use two levels of theory to quantify the intracomplex energy transfer rate in LH2, and find it to be ~30% faster in the membrane, in agreement with experimental results. When accounting for quasi-static variations of the electronic parameters in the LH2 structure, we show that the distribution of the intracomplex transfer rates is broader for the membrane model and suggest that this could reflect a speed-accuracy trade-off commonly seen in biological settings.

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Multiple Quantum-Coherent Energy Transfer Pathways in Photosynthesis: Electronic-Vibrational Mixing within Photosystem II CP43/CP47 Antenna

We investigate how the geometry of buffer networks impacts the protection of quantum coherence in spin clusters that interact with thermal environments. We explore all buffer networks that can be embedded in a plane and find that the connectivity of the buffer network is crucial in determining the protection time of quantum coherence in a single central spin. Our results indicate that the maximal planar graph provides the longest protection time for a fixed number of buffer spins. However, increasing the number of buffer spins does not always lead to longer protection times [1]. With the help of a quantum master equation [2], our simulations show that a tetrahedral geometry of a four-spin buffer network offers the most optimal protection against environmental effects. These findings could help us to better understand biochemical processes since we frequently observe tetrahedral geometry in natural molecules [3].

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Electron Transport in Proteins: A Theoretical Investigation

Proteins have been identified as promising building blocks for the development of novel electronic devices due to their unique properties. Conductance measurements across proteins have revealed remarkable characteristics, such as a conductance in the nanoSiemens range, nearly temperature-independent behavior, low decay with increasing protein size, and dependence on the orientation of the protein relative to the attached electrodes.

These findings have stimulated the creation of theoretical models to explain the electron transport mechanism through proteins, including the hopping model, various tunneling models, and the flickering resonance model. However, developing a comprehensive theory remains challenging, mainly due to the observation of varying conductance behavior under different experimental conditions.

To address this issue, our research group proposed a novel theoretical framework based on a generalized Landauer formula and a quantum master equation. The aim of this new approach is to explain the observed conductance properties of proteins and to make predictions for the outcomes of future experiments without relying on high-performance computing. Our study provides new insights into the electron transport mechanism across proteins, which could be useful in the design of innovative protein-based electronic devices. Moreover, our findings could also have implications for the development of new bio-inspired materials and devices with unique properties.

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Quantum Control of Radical Pair Dynamics beyond Time-Local Optimisation

By adapting Gradient Ascent Pulse Engineering (GRAPE) to optimise reaction yields, we realise arbitrary waveform-based control for spin-selective recombination reactions of radical pairs in weak magneticfields. Our approach overcomes drawbacks of earlier attempts [1] at realising reaction control of radical pair dynamics obtained with time-local optimisation techniques, which did not allow for coherent control of complex radical pair spin systems showcasing magnetic field effects exclusively in the low field regime, due to using a simplified high field approximation. We demonstrate how efficient time-global optimisation of the radical pair recombination product yields can be realised by gradient based methods in combination with time-blocking, sparse sampling of the yield, and evaluation of the central single-timestep propagators and their Frech´et derivatives using iterated Trotter-Suzuki splittings. We show results for a toy model, previously used to demonstrate coherent control of radical pair reactions in the simpler high-field scenario, and for a realistic exciplex-forming donor-acceptor system comprising a total of 16 nuclear spins in weak magnetic fields. This raises the prospect of spin-controlling reaction yields of actual radical pair systems in ambient magnetic fields. In this way, our study paves the way for applications of quantum control to biological radical pair reactions, to suppress/boost radical pair reaction yields using purpose-specific radio-frequency waveforms, and for reaction-yield-dependent design principles for quantum magnetometry and noise resilient qubit architectures.

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Investigation of kinetic and magnetic isotopic effects of D20 in neuronal voltage-gated ion channels

Voltage-gated ion channels (VGCs) are highly specific voltage sensitive transmembrane proteins translocating specific ion species such as Na+, K+ and Ca2+ and regulating their exchange in excitable cells. In the central nervous system, they are responsible for the generation and shaping of the action potential, the main mean of neuronal communication. In addition to their central role in neuronal physiology, VGCs are gaining increasing importance in clinics, as structural mutation or functional abnormalities in these transporters have been linked to numerous dysfunctions including mood disorders, chronic pain, hypertension, neurodegeneration, and cancer. Yet, the mechanisms underlying ion transportation have not been thoroughly explained, and classical models based on coulombic interactions failed to successfully account for the remarkable values of translocation and specificity found experimentally. Consequently, alternative models including the contribution of non-trivial quantum phenomena have been proposed. Recent computational studies found ion transportation rates to be highest when the channel oscillated between alternating states of coherence and decoherence. Further, simulations of ion transport through the channels pore showed the ions themselves to be close enough between them to be described as in a state of quantum superposition, and thereby consistent with wave-like propagation through the channel. As the relative impact of quantum feature on ion translocation could be enhanced by the particular electromagnetic sensitivity of VGCs, we decided to assess the contribution of kinetic isotopic effects (KIEs) on neuronal VGCs currents, through partial deuterium oxide (D2O) replacement, alone or in combination with exposure to extremely low frequency electromagnetic fields (ELF-EMFs), resembling the endogenous electromagnetic field produced by neuronal activity in the brain, to investigate a possible synergistic effect between the electromagnetic properties of neuronal membrane and the coherent state of VGCs. A 50 % replacement with D2O significantly decreased the current amplitude and delayed the activation of both Na+ and K+ VGCs in a reversible manner. This effect was not imputable to relative changes in pH and viscosity, suggesting the presence of a KIE on VGCs conductance. Acute exposure to 0.5 mT 50 Hz ELF-EMFs did not produce significant effects on current amplitudes or activation times. However, it interestingly abrogated the impact of D2O replacement on sustained K+ currents, suggesting the presence of magnetic isotopic effects that shed a light on the role of the electromagnetic homeostasis in the regulation of ion transportation.

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Investigating the Intercalation of Cryptolepine between DNA Watson and Crick Base Pairs

Cryptolepine, a natural drug produced by the Cryptolepis Sanguinolenta plant, is known for its anti-malarial properties [2, 1]. Unfortunately, it is also believed to have cytotoxic properties, making its use to treat malaria in humans difficult [2]. Despite this, interest in Cryptolepine's properties for cancer treatment has sparked interest in further investigation, in particular, we perform computational work on the Cryptolepine's ability to intercalate between cytosine rich sequences in DNA. We seek to understand the mechanism with which the molecule binds between DNA base pairs, specifically cytosine and guanine bases. We also seek to investigate which sites it favours as experimental data suggest that Cryptolepine prefer to bind within certain base pair combinations. This has been investigated by performing DFT calculations using the B3LYP XC-functional and the 6-31g basis set for the DNA with and without the backbone structure. As the Cryptolepine is believed to be stable between the DNA bases via long range interactions throughπ−πinteractions, Molecular Orbital analysis has also been used to investigate the HOMO and LUMO structures of the Cryptolepine-DNA complex. The GD3 correction has been applied to the DFT calculation. We perform molecular dynamics calculations of a DNA structure with explicit water solvent which demonstrate the ability of Cryptolepine to bind within DNA base pairs in biological conditions and combine this with steered MD as well as QMMMmethods to investigate the structure as it enters and leaves the DNA base pairs. Cryptolepine's ability to bias towards certain sites in DNA could play a pivotal role in assisting with cancer treatment with its ability to potentially block it from replicating.

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Role of environmental factors in quantum coherent exciton transport in LH2

It has been proposed that photosynthetic complexes, such as LH2, exploit quantum coherence in order to facilitate energy transfer of excitations and that environmental degrees of freedom are a key component to its ability to maintain long lived coherences. Experimental studies generally will isolate the LH2 in a detergent solution, shedding it of its membrane. Recent experiments have however reported differences in optical signatures for LH2 in detergent, and embedded in a membrane, indicating that the membrane may serve an important role in energy transfer. We apply the hierarchical equations of motion framework in order to accurately simulate energy transport and excitonic coherence properties of the LH2 complex, comparing the results for the two different models that represent LH2 in detergent, and embedded in a membrane. This in turn highlights the importance of preserving the complexes native environmental factors in order to study the functional role of coherence within the complex.

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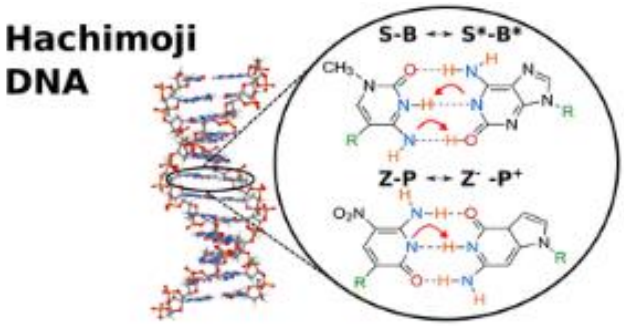
Energy and Charge Dynamics in the Photosystem II Reaction Center

DNA is one of life's most fundamental building blocks due to its ability to encode for the construction of cells and proteins. While the structure proposed by Watson, Crick, and Franklin is a successful model, they fail to address why only four bases are used throughout nature (A, T, C and G) [1]. Work done by Schrödinger defines the structural conditions for DNA to be able to encode information and undergo Darwinian evolution. However, other molecules also meet these structural requirements but are not seen in nature [2, 3]. Hachimoji DNA is a synthetic nucleic acid extension of DNA that proposes an additional four bases (Z, P, S and B) [4]. The additional bases follow Schrödinger's conditions to sustain life but are not seen in nature [2, 3, 4]. We investigate the properties of hachimoji DNA and probabilities of proton transfer between hachimoji bases. First, we construct a scheme of possible proton transfer reactions which could lead to the breakdown of the base pairing rules, analogous to work proposed by Löwdin [5]. We have determined that the reaction barriers in hachimoji DNA are adequately low for proton transfer to occur at biological temperatures. We also show that the proton transfer is much more likely to occur in hachimoji over normal DNA, as the reaction barriers in Z-P and S-Bare 30% lower than those in C-G and A-T. Suggesting the frequency of proton transfer in hachimoji DNA is higher than canonical DNA, which can lead to mutations [6].



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NIR light induces senescence in cancer but not healthy cells

The application of near infrared (NIR)-light to living systems has been suggested as a potential method to enhance tissue repair, decrease inflammation, and possibly mitigate cancer therapy-associated side effects. In this study, we examined the effect of exposing three cell lines: breast cancer (MCF7), non-cancer breast cells (MCF10A), and lung fibroblasts (IMR-90), to 734 nm NIR-light for 20 minutes per day for six days, and measuring changes in cellular senescence. Positive senescent controls were induced using doxorubicin. Flow cytometry was used to assess relative levels of senescence together with mitochondria-related variables. Exposure to NIR-light significantly increased the level of senescence in MCF7 cells (13.5%; $P<0.01$), with no observable effects on MCF10A or IMR-90 cell lines. NIR-induced senescence was associated with significant changes in mitochondria homeostasis, including raised ROS level (36.0%; $P<0.05$) and mitochondrial membrane potential (14.9%; $P<0.05$), with no changes in mitochondrial Ca2+. These results suggest that NIR-light exposure can significantly arrest the proliferation of breast cancer cells via inducing senescence, while leaving non-cancerous cell lines unaffected.

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Effect of Lithium Isotopes on Sodium/Lithium/Calcium Exchanger in Mitochondria

Lithium (Li), ingested in the form of simple Li carbonate or citrate salts, has been used as the forefront treatment of bipolar disorder for nearly fifty years [2] but, surprisingly, the mechanism of Li action remains poorly understood. Li has two stable isotopes which have been shown to affect animal behavior [3, 4] and electrical response in neuronal tissues [5]. To further explore the action of Li isotopes we study mitochondrial transmembrane protein (ion exchanger) – sodium/lithium/calcium exchanger (NCLX) as it has been proposed as a molecular target for Li+ ion [6].

The goal of this research is to find if Li isotopes enter mitochondria differently through the NCLX. To study this question we used two methods: (i) calcium-induced fluorescence [7] to monitor the dynamics of Ca2+ efflux in presence of different Li isotopes and (ii) inductively coupled plasma mass spectrometry (ICP-MS) [8] to study the transport of Li isotope through mitochondrial membrane by measuring the ratios of Li isotopes inside and outside mitochondria.

As expected, it was shown that there is a difference in Ca dynamics in presence of either Li, Na or K in case of functional NCLX. In case of Li isotopes, it was shown that there is no difference between Li isotopes partitioning in heart mitochondria as well is no detectable difference between two isotopes in Ca efflux with or without inhibition of NCLX. These results suggest that there is no different isotopic effect on NCLX or NCLX is not the only one molecular target for Li.

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Spectroscopic Analysis of Fluorescence Quenching and Energy Transfer Dynamics in Fluorescent Proteins

Fluorescence quenching is a physicochemical process that causes the decrease in fluorescence intensity of a fluorescent sample. This process has become an important tool to determine the activation status of proteins, nucleic acids, and membrane systems in biology [1]. The impact of fluorescence quenching on protein-protein interactions is not fully understood [2]. Thus, further research is needed to develop our understanding of the effect of quenching on the dynamical processes which occur within fluorescent biological samples. In this study, we report the spectroscopic analysis of fluorescence quenching and energy transfer dynamics in monomeric Enhanced Green Fluorescent Protein (mEGFP), dimeric EGFP (dEGFP) tandem dimer, and Discosoma Red Fluorescent Protein (DsRed), with the external collisional quenchers of potassium iodide (KI) and copper sulfate (CuSO4). The experiments were carried out using steady-state and time-resolved fluorescence spectroscopy on fluorescent protein assemblies with varying quenching concentrations. Our results explore whether the addition of external quenchers will induce additional dephasing factors between the system and the environment.

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Investigating Lithium Isotope Effects in HT22 Neuronal Cells

Lithium has been used as a treatment for bipolar disorder since the mid 20th century. Ubiquitously found in nature, lithium is composed of two stable isotopes: 92.41% ^{7}Li and 7.59% ^{6}Li. There is some research that indicates these two isotopes of lithium may have differential effects on rat behaviour and neurophysiology. For example, an early work found the general activity level of ^{6}Li-treated rats to be 50% lower than ^{7}Li- treated rats for a same dosage, and more recently a differential effect of lithium isotopes on activity in a ketamine-induced model of mania in rats was reported. The observed differences between the lithium isotopes may be due to their difference in mass or through quantum mechanisms as each isotope has a different nuclear spin state. While there are multiple hypotheses by which lithium isotopes may modulate behaviour and neurophysiology, biochemical and cellular pathways including GSK-3-β kinase activity may be a possible target for lithium isotope effects. In this work using the mouse hippocampal-derived HT22 cell line, we have evaluated lithium isotope effects in four tests: neuronal cell viability, GSK-3-β phosphorylation, GSK-3-β kinase activity, and intracellular isotope uptake. Using ICP-MS, we were able to detect both lithium isotopes in cell lysates in order to test differences in Li isotopes uptake by the cells. We report that both lithium isotopes inhibited GSK-3-β activity and increased GSK-3-β S9 phosphorylation as expected, were not toxic to the cells and were able to enter the HT22 cells from the buffer solution. However, we report no significant difference between lithium isotopes in any of these experiments.

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Visualizing Pre- and Post-Reaction Quantum Correlations in the DNA-EcoRI Catalytic Complex

Long-range electronic dispersion correlations are instrumental in the synchronized cleavage of double-stranded DNA by specialized enzymes called type II restriction endonucleases. Such enzymes—including EcoRI, the first identified in Escherichia coli—bind catalytically to spatially separated nucleotides via sequence-specific, DNA-targeting enzymatic subunits. EcoRI, which does not require ATP or other chemical energy currency to function, is observed to activate through "assistance" from the DNA substrate. It has been proposed that many-body electronic correlations across the entire complex mediate the synchronized catalysis [P. Kurian et al., J. Theor. Bio. (2016)], with EcoRI creating a decoherence-free subspace for its DNA target during the double-strand cleavage. A rigorous model, however, remains to be developed for the entangled electrons in the complex, in which two distant (>20Å) phosphodiester bonds are cleaved in concert by coordination with divalent metal cations (e.g., Mg2+). The role of quantum electronic fluctuations of these ions, the surrounding aqueous solution, enzyme residues, and DNA bases have yet to be accounted for within the existing model for DNA-EcoRI synchronized cleavage. To support the analysis of collective many-body dispersion eigenmodes [M. Gori et al., arXiv:2205.11549, in review with Phys. Rev. Lett. (2022)] associated with the complex, a series of realistic pre- and post-reaction state DNA-EcoRI complex configurations with Mg2+ and Mn2+ were constructed to examine its ligand- and configuration-dependent electronic fluctuations. Molecular dynamics simulations with GROMACS enabled the generation of non-equilibrium configurations for said complex states, providing a controlled computational environment to perform accurate quantum chemical analysis and ascertain a more complete understanding of the multipartite entanglement that contributes to the observed correlations in double-strand catalysis.

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Quantum tunnelling in methylated DNA

Methylation is an important process of gene regulation in DNA, which means that the methylation of specific sites of the nucleotides behaves as a signalling for gene expression [1]. Nonetheless, this process can also occur in unintended sites due to the presence of other alkylating agents in the cells that derive from external sources, such as smoking and pollutants [2]. This type of structural change may be implicated in DNA mutations during the process of replication, and if not promptly accounted for by DNA repair mechanisms, may lead to the development of diseases like cancer.

One common example of an alkylating agent is dimethyl sulfate (DMS), which can methylate guanine in the O6 position, giving origin to O6-MeG, considered highly mutagenic. Due to a steric competition in the binding site of double-strand DNA, this purine can pair with thymine, causing a point mutation in DNA [3], or correctly with cytosine but with a missing hydrogen bond [4].

We suggest that not only the tautomerization of base pairs can be an important cause of mutations in DNA, but that tunnelling through the energy barrier of the reaction may also play a part in this phenomenon [5, 6]. Hence, we explored, from a quantum chemical point of view, if the methylation of DNA modifies the probability of tautomerization, and what are the mechanisms behind this process.

We performed DFT calculations to investigate the optimal structures of the O6-MeG-C and O6-MeG-T base pairs and their tautomers. Similarly to what we previously reported for relatedsystems, we employed the B3LYP hybrid exchange-correlation functional and the 6-31G** basis set [7, 8]. We will then examine the transition states leading to tautomerization and discuss the importance of tunnelling effects in these systems. We will extend the calculations to explicitly account for the solvent and local environment through QM/MM calculations.

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Theoretical calculation of the TPPS4 aggregates formation

Porphyrins are cyclic compounds formed by the linkage of four pyrrole rings through methine groups. Recently, 5,10,15,20-tetrakis(4-sulfonatophenyl) porphyrin (TPPS4) molecules have been extensively studied because they efficiently self-associate from monomers to large J- or H- aggregates in aqueous media depending on the compound concentration and on pH value. Molecular packing in the aggregates is still not clear, while, according to properties of photosynthetic pigment protein complexes, molecular aggregation is the main factor influencing various spectral properties. We investigate TPPS4 aggregation process by designing small molecular complexes and studying their properties using theoretical modeling. The aim of this study is to determine the possible stable TPPS4 dimers and larger aggregates.For the quantum-mechanical (QM) subsystem DFT B3LYP/6-311G(d,p) was used. The most stable zwitterionic Z1 structure is shown in Fig. 1. A general AMBER force field (GAFF) was extended to support Z1 molecule. J-dimer was constructed from the parameterized monomer. TPPS4 dimer was put into box filled with explicit water molecules. Molecular dynamics (MD) minimization, heating and equilibration of this dimer were done. Dimeric form of the TPPS4 dimer was found to be stable in aqueous solution at room temperature.

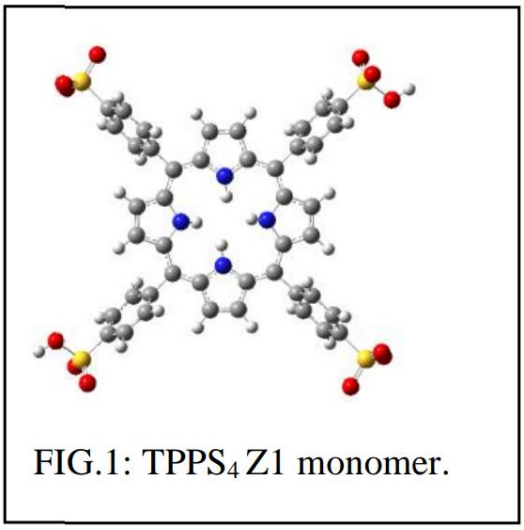

FIG.1: $TPPS_4$ Z1 monomer.

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From Driven Radical Motion Towards Live Magnetosensing

The mechanism of magnetoreception is one of the grand puzzles of modern science. One leading hypothesis suggests that its explanation might lie in a radical-pair within the protein cryptochrome (CRY) that acts as a magnetic field sensor by utilising quantum coherent spin dynamics and spin-selective recombination reactions [1]. Whilst the underlying principles of this radical-pair mechanism (RPM) are well understood and can explain many fundamental traits of a compass sense, there remains a significant question as to how radical-pairs in CRY can deliver the required sensitivity in a noisy biological environment. In particular, it is known that spin relaxation, inter-radical interactions, such as the electron-electron dipolar (EED) interaction [2], and a large number of coupled nuclei (hyperfine interactions), can severely widen the sensitivity gap between model predictions and required sensitivity for a reasonable signal accumulation time in animals.

Here, I will demonstrate that radical motion [3, 4], in the form of harmonic driving of the inter-radical distance, can help to close this sensitivity gap in the presence of inter-radical interactions, by enhancing and restoring magnetosensitivity through Landau–Zener–Stuckelberg–Majorana transitions. I will discuss potential sources of this radical motion arising as an inherent element of the biological environment in live magnetosensors. Lastly, I will motivate the need for model treatments accounting for realistic biological conditions by considering the importance of the number of coupled nuclei and inter-radical interactions in investigations of quantum coherence [5] and the optimality of compass precision as assessed by the quantum Fisher information [6, 7].

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Thermalization of open quantum systems using variational approach

In wavefunction-based simulation approaches of open quantum systems, maintaining precise representation of the bath as a constant temperature thermostat is challenging, because energy exchange between the system and the bath changes thermal properties of the finite-sized bath. Generally, a larger number of explicitly modelled QHO modes must be included to minimize effects of thermal energy accumulation in the bath, however, it can be numerically expensive. Therefore, one must always balance between the size of the model, accuracy of the chosen numerical method and its numerical cost. Alternatively, one could try to numerically change wavefunction variables during numerical propagation in a way as to prevent the accumulation of thermal energy in the bath and to maintain it at a desired temperature, i.e., to perform thermalization.

In this work we design thermalization algorithm for the numerically exact multiple-Davydov D2 trial wavefunction for simulation of relaxation dynamics and spectroscopic signals of open quantum systems using the time-dependent Dirac-Frenkel variational principle. By applying it to the molecular aggregate model, we demonstrate how the thermalization approach allows to significantly reduce numerical cost of simulations by reducing the number of oscillators needed to explicitly simulate aggregate's environment fluctuations, while maintaining correspondence to the exact population relaxation dynamics. Additionally, we demonstrate how thermalization can be used to find the equilibrium state of the electronically excited aggregate state, necessary for simulation of fluorescence and other spectroscopic signals.

The presented thermalization algorithm creates opportunities to investigate larger system-bath models than was previously possible using the multiple-Davydov D_2 trial wavefunction

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Quantum Brownian Motion in the Caldeira-Leggett Model with a Damped Environment

We model a quantum system coupled to an environment of damped harmonic oscillators by following the approach of Caldeira-Leggett and adopting the Caldirola-Kanai Lagrangian for the bath oscillators. In deriving the master equation of the quantum system of interest (a particle in a general potential), we show that the potential is modified non-trivially by a new inverted harmonic oscillator term, induced by the damping of the bath oscillators. We analyze numerically the case of a particle in a double-well potential, and find that this modification changes both the rate of decoherence at short times and the well-transfer probability at longer times. We also identify a simple rescaling condition that keeps the potential fixed despite changes in the environmental damping. Here, the increase of environmental damping leads to a slowing of decoherence.

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A Quantum Compass From Superoxide Close to FAD- an impossibility! Or is it...

The remarkable navigational capability of migratory birds is thought to be enabled by the spin-dependent quantum dynamics of radical pairs situated within the flavoprotein cryptochrome. The direction of the Earth's magnetic field (50µT) alters the reaction yields of these radical pair dynamics, informing the birds' innate compasses [1]. The efficacy of the avian magnetic compass strongly depends on spin-spin interactions and the lifetime of spin state coherences within radical pairs. Inter-radical interactions such as electron-electron dipolar coupling can prove detrimental to both the magnetosensitive spin evolution and the preservation of the associated coherences. This is particularly relevant to the proposed radical pair of superoxide and FAD, [$FADH^{\bullet}O_2^{\bullet -}$], whose proximity within the protein cryptochrome would result in extraordinarily strong dipolar coupling and suppressed magnetosensitivity [2]. This was implicated in recent experimental studies positing a dark-state magnetic field effect [3]. We here demonstrate that this can be counteracted by leveraging the quantum Zeno effect, employing strongly asymmetrical recombination rates from the singlet-triplet spin state interconversion in the radical pair [4, 5].

Making use of the Nakajima-Zwanzig equations of motion, a predictor of compass sensitivity has been calculated for different recombination and decoherence rates for this narrowly separated hypothesised radical pair [6]. This has indicated that a recovery in sensitivity is possible when the system exploits the quantum Zeno effect, hence bolstering the claim that significant magnetic field effects can be achieved with a superoxide in close proximity to FAD. The enhancing effect relies on establishing close degeneracy of energy levels in the effective Hamiltonian (the generator of the system motion in the presence of spin dependent recombination) in addition to the usual Zeno scaling of the lifetime.

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Organic synthesis of deuterated oligonucleotides for neutron diffraction studies

ABSTRAC DNA mutations are formed due to exposure to radiation and mutagenic chemicals or with no known contributing factor, referred as spontaneous mutations. These types of mutations arise from tautomerisation (movement of the positions of hydrogen atoms) of the bases; A, T, G and C which form the DNA nucleotides along with deoxyribose sugar and phosphate group. If the tautomerisation takes place during DNA replication and successfully evades DNA proofreading mechanisms, the mutation gets incorporated into the DNA and can cause cancer and genetic diseases. Many computational modelling studies of this tautomerisation mechanism have been performed but there is scarce experimental evidence for it. We have long-term aims to use neutron diffraction to study, at the atomic scale, the position of protons in DNA and identify the presence of tautomers. However, neutron diffraction suffers from background scattering by hydrogen atoms so for the aim to be feasible, sample DNA must be made which contains entirely deuterium atoms (heavier isotopes of hydrogen which are otherwise chemically identical) instead of hydrogen. The aim of this PhD research is to develop a route to chemically synthesise the building blocks of this DNA – fully deuterated nucleotides using mixture of optimised partial deuteration reactions available in the literature along with protective group chemistry.

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Aggregate Oriented Theory of Internal Conversion Dynamics and Spectroscopy of (Bacterio)Chlorophyll Molecules

The (bacterio)chlorophyll molecules are the light-absorbing pigments of the majority of natural light-harvesting systems on Earth. The aggregation of the pigments into the photosynthetic antennae modulates and extends the useful absorption spectral width by connecting different spectral regions, and it provides a spatial connection between absorption locations. In both spectral (energy) and spatial domains, the aim is to deliver the energy toward the reaction center. So far, in most of the antenna models, the (bacterio)chlorophyll and related pigments were considered as two-electronic-level systems. The current interest in studying photosynthetic systems spectroscopically has shifted towards the influence of intramolecular vibrational modes on the spectra (see e.g. [1]) and the excited-state energy transfer (EET) dynamics. There is no reason to believe that the second lowest excited state of the chlorophylls, the so-called Qx state, is less important than vibrational states in modulating the energy landscape of the photosynthetic antennae. Moreover, it is likely that there is a vibronic coupling between the Qx and Qy states [2] which makes the extended model of the pigments interesting from the point of view of their vibrational structure and dynamics. We calculate the absorption spectra and internal conversion dynamics of a model chlorophyll molecule comprising the Qx and Qy states and two explicit vibrational modes coupling the two electronic states to each other. We apply the methodology compatible with the existing studies on aggregates, i.e., the effective description of the protein environment by its spectral density. We optimize the parameters to fit experimental spectra measured in different solvents and environments. We attempt to identify parameter manifolds that lead to identical absorption spectra to prepare the ground for simulating more information-rich spectroscopic data. In certain parameter regions, the model predicts mixing between Qx- and Qy-related vibrational states which is potentially accessible to quantification by polarization-specific spectroscopies. Optimized pigment models should serve as building blocks to construct more involved models of the photosynthetic antennae and the reaction center, in order to re-evaluate the assignments of various spectral features in the multidimensional vibrationally sensitive spectra [1].

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Investigation of energy transfer in isotopically-labelled bacterial photosynthetic systems

Light harvesting complexes in nature exhibit the remarkable ability of transferring excitons ultrafast and over long distances without dissipation into the environment. Most importantly, this very high efficiency is achieved despite the non-crystalline order and dynamic movement of these proteins. On the contrary, it has been proposed that the vibrational motion of the protein scaffold assists in the energy transfer by preventing decoherence and making use of the quantum properties of the exciton, such as delocalisation. In order to test this hypothesis, our project aims to alter the vibrations of the LH2 protein in the bacterium *Rhodobacter sphaeroides* by changing the carbon atoms with the heavier isotope carbon-13, in order to detect potential differences in their energy transfer dynamics. Understanding the underlying mechanism of this process can prove beneficial in the design of artificial solar cells, but also in avoiding decoherence during quantum computation. Our preliminary results on the successful incorporation of carbon-13 in the protein and the accompanied vibrational shifts observed will be presented and discussed.

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Quantum Mechanical Approach in Drug Activation: Case(Isoniazid)

Isoniazid (Isonicotinic acid hydrazide, INH) is one of the oldest synthetic drugs. It has been used as the frontline treatment of tuberculosis (TB) caused by *Mycobacterium Tuberculosis* (Mtb) since 1950s. INH is oxidised in the cell walls of Mtb bacteria by the catalase-peroxidase enzyme KatG to form the isonicotinoyl radical (NAD•), which can react with NAD(H) to form the enzyme-inhibitory INH-NAD adduct.[1] This adduct inhibits the action of the enzyme 2-trans-enoyl-acyl carrier protein reductase or InhA, which is involved in mycolic acid biosynthesis.[2] We hypothesise that a radical pair mechanism is involved in the formation of this INH-NAD adduct. The goal of this project is to investigate whether we can detect a magnetic field/ isotope effect as evidence that the drug action is indeed mediated by quantum coherent spin dynamics to generate InhA inhibitors i.e., INH-NAD(H) adducts.

INH and isotopically-substituted INH was activated both non-enzymatically[2], by oxidation with Mn(III) and also enzymatically with KatG, in the presence or absence of a magnetic field. The products, separated by HPLC and characterized by mass spectrometry, and will be described.

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