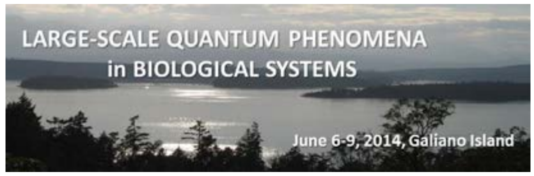


# TALKS: TITLES & ABSTRACTS

## M. Berciu: **Polarons: new methods and new paradigms**

We present a variational method, known as the momentum average approximation, which has been shown to provide an accurate yet efficient way to study polaronic problems. Its success is gauged by comparing its predictions against numerically exact results, where available, for different kinds of polaronic hamiltonians. A new paradigm of polaronic behavior is shown to hold in systems where the bosons modulate the particle's hopping integrals.

## E. Bittner: **Quantum Olfaction**

## H. Brown **How trees defy gravity: remarks on the theory of the ascent of sap**

The ability of trees to suck water from roots to leaves, sometimes to heights of over a hundred meters, is remarkable given the absence of any mechanical pump. In this talk I deal with a number of issues, of both a historical and conceptual nature, in the orthodox Cohesion-Tension (CT) theory of the ascent of sap in trees. The theory relies chiefly on the exceptional cohesive and adhesive properties of water, the structural properties of trees, and the role of evaporation (‘‘transpiration’’) from leaves. But it is not the whole story. Plant scientists have been aware since the inception of the theory in the late 19th century that further processes are at work in order to ‘‘prime’’ the trees, the main such process – growth itself – being so obvious to them that it is often omitted from the story.

## A. Buchleitner **Transport on network-like structures: from light harvesting to boson sampling**

I will report some recent results on excitation transport models for photosynthetic light harvesting, and on multi-photon interferences in beam splitter arrays. Depending on the desired format, I could also offer a more general discussion of scaling issues in "complex" quantum systems (including aspects of entanglement spectral theory).

## G. Fleming **Quantum Dynamics in Photosynthetic Light Harvesting**

In this talk I will give an overview of the current experimental and theoretical understanding of the role, origin and importance of quantum effects in natural photosynthetic light harvesting. I will try to point out the areas where questions remain and new experiments and theory are needed.

## B. Green: Quantum Effects and Light-harvesting from the Algal Cell's Point of View

With respect to any cellular structure or function of a liviing cell, the Three Big Questions are:
(1)How does it work?
(2)How did it get that way?
(3)Does it matter?

To set the stage, I will review bacterial and eukaryotic light-harvesting systems, most of which evolved independently and represent different solutions to the problem of harvesting light. The evolution of these antennas did not happen in isolation, but was linked to the evolutionary history of their owners' cells, which were impacted by several levels of endosymbiosis and multiple gene transfers. The soluble phycobiliprotein antenna of cryptophyte algae is an excellent example of the many evolutionary mechanisms involved in the invention of a novel light-harvesting system. The most common form of this antenna, called the "closed" form because of its compact structure, demonstrates quantum coherence, but the genus Hemiselmis has another form ("open") which does not. However, under high light Hemiselmis can express other genes which encode the "closed" form. This raises the possibility that quantum behavior can be switched in response to environmental conditions.

## P. Hore Chemical magnetoreception: the quantum biology of cryptochromes

Migratory birds travel spectacular distances each year, navigating and orienting by a variety of means, most of which are poorly understood. Among them is a remarkable ability to perceive the intensity and direction of the Earth’s magnetic field. Biologically credible mechanisms for the sensing of such weak fields (25-65 microtesla) are scarce and in recent years just two proposals have emerged as frontrunners. One, essentially classical, centres on iron-containing particles. The other relies on the magnetic sensitivity of short-lived radical pairs formed by photoinduced electron transfer. This model began to attract interest following the proposal that the necessary photochemistry could take place in the bird’s retina in specialised photoactive proteins called cryptochromes. The coherent dynamics of electron-nuclear spin states of pairs of radicals is conjectured to lead to changes in the yields of reaction products even though the Zeeman interaction with the geomagnetic field is more than six orders of magnitude smaller than the thermal energy kT. I will outline some of the experimental evidence for the cryptochrome hypothesis, discuss the interpretation of the reported effects of weak (nanotesla) radiofrequency fields on the magnetic orientation of European robins, compare the magnetic responses of various members of the cryptochrome family of proteins, and comment on the extent to which cryptochromes are fit-for-purpose as magnetoreceptors.

## H. Neven Neuroreceptor Activation by Vibration-Assisted Tunneling

G protein-coupled receptors (GPCRs) constitute a large family of receptors that sense molecules outside of a cell and activate signal transduction pathways inside the cell. Modeling how an agonist activates such a receptor is important for understanding a wide variety of physiological processes and it is of tremendous value for pharmacology and drug design. Inelastic electron tunneling spectroscopy (IETS) has been proposed as the mechanism by which olfactory GPCRs are activated by an encapsulated agonist. In the work presented in this talk we apply this notion to GPCRs within the mammalian nervous system using ab initio quantum chemical modeling. We found that non-endogenous agonists of the serotonin receptor share a singular IET spectral aspect both amongst each other and with the serotonin molecule: a peak that scales in intensity with the known agonist activities. We propose an experiential validation of this model by utilizing lysergic acid dimethylamide (DAM-57), an ergot derivative, and its isotopologues in which hydrogen atoms are replaced by deuterium. If validated our theory may provide new avenues for guided drug design and better in silico prediction of eﬃcacies.

## P.C.E. Stamp **Modeling Coherence, decoherence, and quantum relaxation**

A lot of the discussion of coherence effects in biology involves comparison between theory and experiment; but decoherence and quantum relaxation are notoriously difficult to model in systems where interactions are not weak. I start by comparing oscillator bath and spin bath models, and show that the correct decoherence and relaxation dynamics is often very different from that given by standard calculation schemes. These results suggest interesting new possibilities for light-harvesting and magnetoreception systems.

## L. Turin **Electron Spin Changes During Anesthesia in Drosophila**

The volatile general anesthetics Xe, SF6, N2O and CHCl3 cause rapid increases of different magnitude and time course in the electron spin content of Drosophila. With the exception of CHCl3 these changes are reversible. Anesthetic resistant mutant strains of Drosophila exhibit a different pattern of spin responses to anesthetic. In two such mutants the spin response to CHCl3 is absent. We propose that these spin changes are caused by perturbation of the electronic structure of proteins by general anesthetics. Using Density Functional Theory, we show that general anesthetics perturb and extend the HOMO of a 5-residue alpha helix. The calculated perturbations are qualitatively in accord with the Meyer-Overton relationship and some of its exceptions. We conclude that there may be a connection between spin, electron currents in cells and the functioning of the central nervous system.

## V. Vedral **How to measure quantum macroscopicity?**

Measures of quantum correlations are well developed and understood in a wide range of systems, including large many-body systems. They have even been applied to biological energy flow. I plan to briefly discuss measures of entanglement and discord. However, according to the commonly accepted view, it is the GHZ (or the "cat") states that are considered most quantum macroscopic (even though they contain very little entanglement). I would like to explain how quantum macroscopicity is measured and then discuss various experiments in the light of this measure. Finally, I will speculate on whether biological processes can really ever lead to quantum macroscopicity.

## F. Wang **Are There Quantum Effects in Human Perception?**

## J. Werren **When will biological adaptations be "optimal" enough to reveal Q processes?**

Two topics will be covered in my presentation. The first concerns the forces that constrain how close to a phenotypic optimum a biological system can evolve, a topic that could be relevant to when quantum processes can be detected in biological systems. The second concerns how natural genetic variation evolves in diverging co-adapted gene complexes, and whether this type of variation can be used as a tool for analysis of quantum processes in biological systems.

B. Whaley **Photoactivated biological processes as quantum measurements**

We outline a general framework for describing photo-activated biological reactions as generalized quantum measurements of external fields, for which the biological system takes on the role of a quantum meter. Using general arguments regarding the Hamiltonian describing the measurement interaction, we identify the cases where it is essential for a complex chemical or biological system to exhibit non-equilibrium quantum coherent dynamics in order to achieve the requisite functionality.

W. Wiltschko **Magnetoreception in Birds**

Behavioral experiments with migratory birds revealed three characteristics of the avian magnetic compass: (1) it is an ‘inclination compass’, not based on the polarity of the magnetic field, but the axial course of the field lines, (2) it works spontaneously only in a narrow intensity window which can adapt to other intensities, and (3) it requires short-wavelength light. The Radical Pair-Model of magnetoreception suggests spin-chemical processes in photopigments; it can explain these properties. The model is supported by experimental evidence. Cryptochrome, the suggested receptor molecule, has been found in the eyes of birds, where it is located at the disks of the outer segments of the UV-cones. By immuno-histochemical studies, we could show that it is activated by the wavelengths of light that allow magnetic compass orientation in birds.